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U.S. DEPARTMENT OF COMMERCE, C. William Verity, *Secretary*
NATIONAL BUREAU OF STANDARDS, Ernest Ambler, *Director*

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Abstract

An integrated equilibrium kinetic model is described for treating the chemical solution component of corrosion of (Co,Cr)-based superalloys by the (Na, S, V)-molten salts originating from impurities present in hydrocarbon fuels. Gas phase chemistry and gas phase/condensed phase precipitate interactions are modeled using the NASA-Lewis multicomponent free energy minimization program (CEC). Salt deposition rates are calculated with the aid of a chemical frozen boundary layer (CFBL) program. Solubilities of superalloy components (Co and Cr) are modeled from phase equilibrium data, and rate of solution is described by assuming a very thin steady state oxide film, with formation and dissolution occurring according to a parabolic rate law. A range of steady state corrosion rates can be predicted using this approach which are in general agreement with the range of reported test rig results. Further model development would benefit from additional experimental phase equilibrium data on the system Na_2O-CoO-Cr_2O_3-SO_3-V_2O_5.

I. BACKGROUND

A. The Problem of Hot Corrosion

The phenomenon of hot corrosion has received much attention over the past several decades; the state of our knowledge with regard to metals has been summarized in ref. [1]. Much of the most recent interest has centered on hot corrosion of superalloys, in particular, corrosion of superalloys or superalloy with coatings based on Ni, Co, Cr, Al, and Y. In most boiler and gas turbine applications, hot corrosion of these and other materials is due to the chemical action of fuel impurities such as Na, S and V. When these impurities condense out as salts, mass transport of superalloy components occurs which leads to degradation and removal of material from the superalloy surface, and provides a mechanism for oxidative attack on the alloy constituents. While hot corrosion is essentially a chemically driven process, quantitative chemical models describing this process have not been developed.

Two thermal regimes pertaining to hot corrosion have been distinguished by corrosion engineers and materials scientists working in the area of combustion [2]. Low temperature hot corrosion is apparently limited to 650-750 °C. This form of corrosion is characterized by deep smooth pits with sharp boundaries [ref. 3]; the pits are filled with oxides of Al and Cr. Nickel and cobalt are strongly depleted in the oxide relative to the metal. Typically a thin layer of sulfide occurs intermittently along the oxide/metal interface.

High temperature hot corrosion (alternatively referred to as Type 1 corrosion in ref. [2]) occurs near 900 °C (1600 °F) and is characterized by a thick

porous oxide scale, often containing detached metal particles. The metal/oxide interface is highly irregular and deep penetration of the oxide into the metal occurs. A layer of sulfides may occur near the base of the oxide.

B. Previous Models

Generalized models have been suggested for the simple oxidation of metals, perhaps the most notable being the diffusional model of Wagner [4], which has been supported by the observation of parabolic rate laws for several systems involving pure metals. Hot corrosion models must necessarily consider additional factors relating to the complex multicomponent chemistry and the gradients prevailing at the interfaces between metal, scale, molten salt and gas. Some of the necessary considerations are summarized in ref. [5]. One type of general hot corrosion model is represented by the fluxing models of Goebel and Pettit [6], Rapp and Goto [7] and others. In these models, oxide scale is dissolved by the salt, transported and reprecipitated at another site (typically the salt/gas interface). An alternative model proposed by Hancock [8] involves scale cracking and salt penetration of the metal.

The effects of certain variables known to influence corrosion rates, such as thermal cycling, are difficult to model. By contrast, the equilibrium solution chemistry can be modeled, if basic thermodynamic or phase equilibrium data are available. As an indication of the promise this approach holds, Jones [9] has outlined a qualitative model for low temperature hot corrosion which relates to the effect of P_{SO_3} on the removal of cobalt in the form of

molten cobalt/sodium mixed salts. In addition to P_{SO_3} and the activity of Na_2SO_4, the activity of V_2O_5 has a well known effect on corrosion rates. This has been treated by the statistical model of Rathnamma and Bonnell [10].

C. Goals of the Present Study

Given the complexity of available hot corrosion data, it is not surprising that comprehensive chemical models have not been developed. The present study attempts to isolate and estimate the chemical solution component of the corrosion of Co, Cr based alloys by Na, S, V - containing fuels. This will allow an assessment of the importance of the chemical solution contribution to the over-all corrosion rate.

II. OUTLINE OF MODEL

The model presented here is concerned with the mass transport of the Cr and Co components of the superalloy. A representative commercial superalloy [ref. 11] contains (wt.%): 22% Cr, 71.5% Co, 6% Al and 0.5% Y. Cobalt and chromium are the dominant constituents and effective removal of these components (either mechanically or chemically) must occur for corrosion to be extensive. The Cr component is known to improve corrosion resistance by forming a protective scale. Although present in minor amounts, the Al and Y are also very important; however the manner in which these components improve the corrosion resistance of the superalloy is not fully understood. One suggestion [ref. 12] is that Y and Al serve to make the protective oxide film finer grained (hence less porous) and more adherent. Although the model discussed here is currently limited to consideration of the chemistry of

Co and Cr, it should nonetheless be applicable to the observed corrosion of superalloys.

The present model considers the effects of Na, S and V fuel impurities on corrosion. The essential features of the model treated here are given in Fig. 1, and will be discussed in the following sections of this report. Briefly, the model consists of the following segments:

1. calculation of combustion and wall equilibria
2. calculation of salt deposition rates
3. calculation of salt phase equilibria and CoO, Cr_2O_3 solubilities
4. modeling of CoO, Cr_2O_3 film formation and solution rates
5. estimation of corrosion rates

The model is compared with burner test rig data to give an indication of the utility of the present approach, along with suggestions for follow-up.

III. CALCULATION OF GAS EQUILIBRIA

A. Methodology

As indicated in Fig. 1, the initial requirement for modeling is knowledge of the gas phase chemistry. It is generally possible to calculate the equilibrium species composition of the combustion gases, including the effect of the fuel impurities, if adequate thermodynamic data are available for all significant species. Where precipitation occurs, it is necessary to model the solution process in order to obtain activity data. The most general method currently available for solving the multicomponent equilibrium problem depends on minimizing the Gibbs Energy (G) for the entire system of known possible

species. For systems where many possible species exist, typical of corrosion systems, a variety of computer codes exist which will minimize the Gibbs energy (G) of a gas mixture, possibly in contact with a collection of pure independent phases. Only recently [13,14] have techniques been developed for handling condensed solutions with variable stoichiometry. The basic method consists of solving a set of simultaneous equations for the free energy of the system, subject to the constraint of mass balance. The general solution techniques used do not *a priori* restrict the computation to non-negative amounts for individual species or phases. Thus, the problem must be solved iteratively, eliminating phases with negative amounts. Once convergence of the mass balance at minimum G is obtained, it is then necessary to iterate by selecting alternate phase sets for possible improvement of the free energy minimum, followed each time by iteratively reconverging the mass balance. The process is continued until no alternative phase-set obeying the phase rule can further lower the system free energy.

For the present report, gas/condensed phase equilibrium calculations were completed using a modified version of the NASA-Lewis Research Center multicomponent equilibrium program which is referred to here as the CEC program [15]. The modifications permit the program to properly handle multiple solutions (liquids e.g.) with non-unity component activities. This is particularly important as most of the species expected to be important in hot corrosion are present as trace species in solution, and with the exception of solids, are unlikely to precipitate as pure phases. Although the modified CEC code treats only ideal solutions, Hastie and Bonnell [16] have shown that an ideal solution model can correctly model solutions considered highly

non-ideal when the proper species are included. Although this is yet to be shown true for the CEC database, assuming ideal solution behavior with regard to multicomponent species is an appropriate first step.

Although the modified CEC program is not generally available, and details of the implementation permitting multiple condensed phase mixtures are not available, the general procedure is as described above, and hand checks on a sample run indicate that the various species in solution have the proper thermodynamic equilibrium constant relationships. The program has also been extensively tested at NASA-Lewis. In particular, a number of stability improvements were made particularly for David Taylor Naval Ship R&D Center to permit the program to successfully converge with input specifying one or more atoms of species to be present in parts per million or less concentration.

The modified program uses a similar input structure to that of CEC, using an extensive database of thermodynamic species. The program still selects needed data from that database automatically, relieving the user of the database preparation in simpler cases. The extra mixture(s) beyond the gas phase are specified by including groups of species names, in the familiar INSERT/OMIT format, following an identifier record (eg. SOLN 2) entered right after the REACTANTS records. Although this database formalism, and the method of denoting solution species is relatively much easier for the occasional user, there is a potential problem of some magnitude. The database for CEC represents pure phases, each defined by a polynomial for the Cp function in the temperature region of validity, and heat and entropy terms (see Hastie and Bonnell, [16] for the form of these entries) from which the species Gibbs

energy can be calculated. For a problem where only pure phases are expected, the fact that the database was designed to permit CEC to select the most stable phase at the calculation temperature is desirable. However, in the case of solutions, the modified CEC program continues to substitute the most stable phase, regardless of the fact that it is not appropriate to use; for example, functions for the solid form of a species are used to represent its Gibbs energy in a liquid solution. This problem occurs whenever the liquidus temperature drops below the melting point of constituent species. Substitution of the solid thermodynamic functions progressively over-stabilizes the solution by the $\Delta G(T)$ of melting. This problem is not easily remedied, as the data base entries were not originally fit expecting extrapolation beyond the stability regions. Rather, the intent was best representation of the pure phase stability. This problem is general for database-driven equilibrium codes, and is not unique to the modified CEC code. The code should assume extrapolatable functions, and use the most stable phase matching the state (gas, liquid, solid) of the mixture. Since the majority of calculations for this work, were at temperatures near or above the melting point of all solution species, the calculated equilibria should be close to the true values. In any case, since the effect is to accentuate the stability of the liquid solution, any error in a corrosion estimate based on solution solubilities tends to be conservative.

Another difficulty is that when CEC determines that a solution phase is not stable for a chosen temperature, the solution is removed permanently. The code does not further consider it for lower temperature problems. Since CEC convergence is generally much more reliable working from higher temperatures

to lower, this is a significant problem. It makes impossible the simultaneous calculation of the combustion composition and the downstream (wall) equilibria for simple entry to Chemical Frozen Boundary Layer [CFBL] program described in Section IV.

B. Input Data

i. Fuel and Fuel/Oxidant Ratio

Possible fuel stoichiometries range from $CH_{1.5}$ to $CH_{2.0}$. For turbine applications, a value of $CH_{1.8}$ is typical; for most boiler applications a value of $CH_{2.0}$ may be typical. For purposes of carrying out the model calculations, we have used a value of $CH_{1.8}$; however the effect of varying fuel composition between $CH_{1.8}$ and $CH_{2.0}$ on composition of salts would probably be negligible.

Possible fuel oxidant ratios (fuel: air, by volume) range from 1:10 to 1:100. In practice, typical ratios are near 1:30 for boiler operation and 1:50 for turbines. For the present calculations the main effect of varying the fuel/air ratio would be on P_{O_2}, and on the adiabatic flame temperature. However, for the range of P_{O_2} considered here (see below), the effect of such variations on salt chemistry would probably be insignificant. For purposes of modeling we have used a fuel/oxidant ratio of 1:30; this is equivalent to a fuel-to-oxidant weight ratio of 0.04538, based on a fuel density of 1.38 g/cm^3, typical of kerosene-type turbine fuels. The oxidant used in the calculations corresponds to clean air, with one wt. % water vapor present.

ii. Temperature and Pressure

While flame temperatures may reach 2600 °C during combustion, depending upon heat transfer, fuel/oxidant, preheat, etc., the temperatures of the downstream components subject to hot corrosion range from 600 to 1000 °C. We have selected two temperatures for model calculations: 977 K (1300 °F) and 1177 K (1650 °F). These temperatures approximate the thermal regimes of low temperature and high temperature hot corrosion (~700 and ~900 °C, respectively).

Pressures in operating combustion systems vary widely depending on conditions of mass flow and the system design, but typically turbines operate at pressures above 1 atm. To study the effect of pressure on salt compositions we have completed model calculations at 1, 5, 7, 10, and 15 atm total pressure.

iii. Concentration of Na, S, V in Fuels

Impurity concentrations currently of interest to the Navy are summarized in Table 1, corresponding to "base" fuel, fuel "GT10", and fuel "GT12". To provide a range of impurity concentrations which encompass the fuels in Table 1, we have completed model calculations using the matrix of impurity concentrations in Table 2. Thus sodium contents range from 0.1 ppm (wt.) to 10 ppm; sulfur from 0.01 to 1.0 wt%, and vanadium from 0.1 to 10 ppm (wt). The matrix of fuels represented by Table 2 leads to 27 different impurity compositions. For purposes of ease in referring to these compositions we shall use a nomenclature in which the values of (Na, S, V) respectively are indicated according to the row of Table 2 in which they fall. Thus,

composition (111) represents 0.1 ppm Na, 0.01 wt% and 0.1 ppm V; composition (132) represents 0.1 ppm Na, 1.0% S and 1.0 ppm V, etc.

iv. Thermodynamic Database

The database installed at NASA-Lewis for use with the modified CEC code consists of the latest NASA thermodynamic database (1986), with the addition of an extensive set of metal vanadates, including solid and some liquid vanadates for Al, Sb, Ba, Bi, Cd, Ca, Ce, Cr, Co, Cu, Hf, In, Fe, La, Li, Pb, Mg, Mn, Mo, Nd, Ni, K, Ag, Na, Sr, Sn, Sn, Ti, W, Y, Zn, and Zr, based on an extensive literature search and considerable estimation by workers at Aerodyne under contract to DTNSR&DC, Annapolis. For the model runs reported here, Table 3 gives the species considered for the compositions modeled. The phase notation for all species is given in parenthesis except for the gas phase species.

The most conspicuous missing species in this data base pertinent to vanadium transport is a gas species of V_2O_5 stoichiometry. A general literature survey has been made by JANAF [17], but their critical assessment of the gas phase data has not provided a clear cut vaporization mechanism. It is likely that the vaporization process is incongruent, with a variety of gas species. Although JANAF [17] calculates a "decomposition temperature" of 1963 K at $P_{O_2} \approx 1$ atm for the equilibrium,

$$V_2O_5(\ell) = V_2O_4(\ell) + 1/2\ O_2\,,$$

one or more vanadium oxide species are also major gas species. The literature is quite uncertain regarding the nature of these species, owing to a scarcity

molecular specific (ie. mass spectrometric) studies. It is clear that this system is overdue for careful study, including experiments where the oxygen partial pressure can be controlled to permit measurements in well defined V-O phase regions. The database for CEC supplied to NBS contained the gas species VO and VO_2, but had no entries for what is considered the majority gas species, V_4O_{10} (dimeric V_2O_5). Part of the problem is that there are essentially two groups of measurements, represented by the data of Polyakov [18] at high temperature limit, and the data of Semenov, et al [19]. The mass spectrometric results of Farber, et al [20] are more in accord with the Semenov [19] data, but their results suggest rapid conversion to a lower oxide (probably $V_2O_3(s)$) with V_4O_8 becoming quite important. Fig. 2 shows the relative partial pressures of the various experimental data. CEC calculations performed with the non-solution version using the coefficients of Table 4 indicate that the Polyakov [18] data will cause V_4O_{10} to become the dominant vanadium gas carrier. On the other hand, the Semenov et al [Ref. 19] and Farber et al [20] data indicate that the pressures of VO_2 and V_4O_{10} are comparable in the temperature regime of interest. For the purposes of this project, it was decided that ignoring V_4O_{10} would be as reasonable as including a possibly erroneous value. It is clear that more experimental on the V-O system is warrented. In particular, a mass spectrometric study where the partial pressure of O_2 can be controlled is necessary to ascertain the importance of gas species such as V_4O_8. In any case, an early test of the effect of adding V_4O_{10} to the data base is highly recommended, particularly before the vanadate database is used extensively.

C. Results

Results of CEC equilibrium calculations for fuels with impurity levels of Table 2 under the conditions outlined above are summarized in tabular form in Appendix A. For corrosion modeling important variables are P_{O_2}, P_{SO_3} and mole fractions of the components Na_2SO_4, V_2O_5 and $Na_2V_2O_6$ in the molten salt phase.

i. Oxygen Partial Pressure (P_{O_2})

As examination of the data in Appendix A shows, oxygen partial pressure does not vary significantly under the conditions of the calculations and falls in the range 6.3 to 6.7 x 10^{-2} atm., as would be expected from the large excess of O_2 in the combustion process. P_{O2} is not affected appreciably by increasing the total pressure from 1 to 15 atm.

ii. Sulfur Trioxide Partial Pressure (P_{SO_3})

The equilibrium partial pressures of sulfur dioxide, sulfur trioxide and oxygen are related by the reaction:

$$SO_2(g) + 1/2\ O_2(g) \rightarrow SO_3(g).$$

Thus, it is sufficient to specify either P_{SO_2} or P_{SO_3} along with P_{O_2} to define the sulfur activity in the system. Increasing the total pressure increases the ratio of P_{SO_3}/P_{SO_2}; increasing the temperature has the opposite effect. Increasing the total pressure from 1 to 10 atm. increases the value of P_{SO_3} by about threefold at 1172 K and by one-and one-half to two times 977 K. As would be expected, values of P_{SO_3} vary widely with sulfur content of the fuel, and range from about 3 x 10^{-7} atm for fuel with 0.01 wt% S to about 1.5 X 10^{-4} atm for fuel with 1 wt% S.

iii. Condensed Phase Compositions

The data for the liquid phase in Appendix A have been recalculated to (mole basis):

$$100\% = Na_2SO_4 + Na_2V_2O_6 + V_2O_5 .$$

A plot of the recalculated data is shown in Fig. 3, where it can be seen that essentially the complete range of possible molar ratios is encompassed with regard to these three components. The groupings that occur in Fig. 3 are related to the necessarily limited distribution of fuel impurity ratios considered in Table 2. The labeling in Fig. 3 allows the groupings to be related to Table 2, according to the labeling convention defined above in section III.B.iii. As Fig. 3 contains all the data from Appendix A, the effect of T and P are not clearly delineated. For this reason, Fig. 4 has been included which shows only data for composition (111); it is clear that increasing pressure increases the ratio:

$$\frac{Na_2SO_4}{Na_2SO_4 + V_2O_5 + Na_2V_2O_6}$$

This effect is greatest in increasing from one to two atm. pressure. Increasing the temperature has the opposite effect.

IV. CALCULATION OF SALT DEPOSITION RATES

A. Methodology

Gokoglu et al [21] have developed a chemical frozen boundary layer (CFBL) code for calculation of salt deposition rates on the walls of combustion systems. This code has built-in constants for the properties of the system where combustion is complete and dominated by the reaction

$$CH_{2.0} + 3/2\ O_2 \rightarrow CO_2 + H_2O.$$

The alkali/sulfur species considered in the gas phase (Na system) are: (1) NaOH, (2) Na, (3) Na_2SO_4, (4) SO_2, (5) SO_3, (6) NaCl, (7) H_2S. Work by Rathnamma and Nagarajan [22] supports the contention that the deposition rates for other salts (e.g. $Na_2V_2O_6$, V_2O_5) parallel very closely their relative quantities from the equilibrium calculations. Thus, for the purposes of this work, vanadium salt deposition rates were presumed to be in proportion (relative to the calculated Na_2SO_4 deposition rates) according to their equilibrium concentration in the calculated solution. This is a reasonable working assumption, as the resulting error is less than that due to other modeling assumptions relating to the physical behavior of the wall deposit. Gokoglu and Santoro [23] have recently reported experimental results in excellent agreement with CFBL calculations.

The version of the CFBL code implemented was nearly identical to the version reported by Gokoglu et al [Ref. 21]. In installing the code on the NBS CYBER 855 system, a few instances of attempts to reference undefined variables were encountered. Subsequent examination of the code indicated that zero entries were correct, and thus the code had been performing correctly on its development system, where a reference to undefined storage returns an appropriate zero. The authors were contacted to confirm this. For convenience, and for general use, the corrected version was assembled for use on 8088/8086/80286/80386-based MS-DOS microcomputer systems with floating point coprocessors.

B. Input Data

The CFBL code requires certain input parameters specifying the area of the deposition surface, size of the gas jet, mass flow, etc. These have been chosen to correspond as closely as possible to burner test rigs for which deposition rate data are available. CFBL input parameters are listed in Appendix B.

C. Results

Results of a series of CFBL calculations for nine compositions from Table 2 are given in Appendix B. The compositions chosen reflect the impurity compositions with the highest sulfur content (1.0 wt. %). Phase compositions of the deposited salts are shown in Table 5, along with total deposition rates. It is evident that calculated salt deposition rates vary dramatically, depending upon salt composition.

V. CHEMICAL MIXING

A. Methodology

For many salt systems a simple regular solution model provides adequate description of the mixing properties [24]. For a ternary system minimum input would be thermodynamic properties of the end members and phase equilibrium information on the binary invariant points. As noted, we are interested, for purposes of this report, in solubilities of CoO and Cr_2O_3 in mixtures of Na_2SO_4-V_2O_5-Na_2VO_6 salts. Unfortunately there are not sufficient phase equilibrium data on the limiting binary systems to develop a realistic regular solution model - therefore we have had to assume that with regard to mixtures of CoO, Cr_2O_3, Na_2SO_4, $Na_2V_2O_6$ and V_2O_5, the heats of mixing are zero. This

same assumption has already been noted concerning the CEC calculation of gas/salt equilibria, and may provide a reasonable approximation, since if the proper mixing species are chosen, the enthalpies of reaction will already be accounted for to a large degree in the thermodynamic properties of the components being mixed.

It is important to note that under the range of T, P_{O_2}, and P_{SO_3} considered here, CoO and Cr_2O_3 will be stable relative to their sulfates [25, 26], and therefore the superalloy chemical solution problem may be treated in two stages: (1) formation of an oxide film, and (2) chemical solution of the oxide film in the salt phase. The solubility of CoO and Cr_2O_3 in sodium sulfate and sodium vanadate melts is thus of central importance. Four ternary systems are of interest: $CoO-Na_2O-SO_3$, $CoO-Na_2O-V_2O_5$, $Cr_2O_3-Na_2O-SO_3$, and $Cr_2O_3-Na_2O-V_2O_5$.

B. System $CoO-Na_2O-SO_3$

Deanhardt and Stern [27] have determined the solubility of CoO in molten Na_2SO_4 at 1200 K (727 °C) as indicated in Fig. 5. Solubility varies markedly with A_{Na_2O} and reaches a minimum of about 100 ppm at about $P_{SO_3} = 10^{-7}$, near the minimum P_{SO_3} encountered in our modeling calculations. At the other extreme near $P_{SO_3} = 10^{-4}$ atm, solubility of CoO would be close to 10 wt.%, using the extrapolated portion of the curve in Fig. 5. However the data in Fig. 5 apply to $P_{O_2} = 0.2$ atm., somewhat higher than that prevailing under the modeling conditions used here.

C. System $CoO-Na_2O-V_2O_5$

No experimental data are available for the solubility of CoO in sodium vanadate, based on a comprehensive literature search completed in late 1986.

D. System $Cr_2O_3-Na_2O-SO_3$

Zhang [28] has published data on the solubility of Cr_2O_3 in fused Na_2SO_4 at 1200 K at various oxygen pressures. An extrapolated curve corresponding to 7×10^{-2} atm., the P_{O_2} prevailing under the conditions of the model calculations, is given in Fig. 6. A marked variation in Cr_2O_3 solubility as a function of P_{SO_3}, with a pronounced minimum, is evident in Fig. 6. The minimum is about 100 ppm at a P_{SO_3} of about 10^{-2} atm., a pressure well above the conditions prevailing during our model calculations. The implication of Fig. 6 is that solubility of Cr_2O_3 in Na_2SO_4 is extensive under the range of P_{SO_3} prevailing during the model calculations.

E. The System $Cr_2O_3-Na_2O-V_2O_5$

Of the four ternary phase diagrams needed for oxide solubility, this is the only one for which direct data [29] are available. The 700 and 900 °C isotherms of the Cr_2O_3 saturation surface shown in Fig. 7 apply to highly oxidizing conditions.

F. Estimates of Equilibrium Oxide Solubilities

From Fig. 7, it is apparent that over the range of $V_2O_5/Na_2V_2O_6$ ratios encountered in Appendix A, oxide solubilities do not vary appreciably. Thus to a first approximation at 700 °C, the sodium vanadate melt dissolves about 45 mol% Cr_2O_3 and at 900 °C, it dissolves about 55 mol% Cr_2O_3. If we assume,

based on Fig. 6, that the same holds true for the sulfate melts, then as a very approximate estimate, molten salts in the system V_2O_5-$Na_2V_2O_6$-Na_2SO_4 dissolve about 45 to 55 mole % Cr_2O_3 at equilibrium under the conditions of the model calculations; for the initial stages of model development, 50 mole% will be used a test value. We do not have sufficient data to make an estimate of CoO solubility under the conditions of the model calculations, but this may not be a serious handicap in the early stages of model development, as Cr_2O_3 dissolution is probably a major limiting factor in superalloy attack.

VI. CHEMICAL KINETICS

A. Methodology

Given that Co,Cr oxides are stable relative to sulfates under our model conditions, formation of an oxide film is assumed to be the first step in superalloy reaction:

$$2\ Cr(alloy) + 3/2\ O_2(g) \rightarrow Cr_2O_3(c)$$

$$Co(alloy) + 1/2\ O_2(g) \rightarrow CoO(c)$$

It is assumed that the salt layer is thin, mobile and gas permeable so that the P_{O_2} is everywhere that in the gas, i.e., at about 7×10^{-2} atm. The formation of CoO and Cr_2O_3 layers is than assumed to occur according to a simple parabolic rate law:

$$(M/A)^2 = kt,$$

where M is mass, A is area, t is time and k is the parabolic rate constant. It is further assumed that solution of the oxide in the available salt is a relatively rapid process, by comparison with film growth. This seems reasonable given the highly fluid nature of the salt melts, and the under-saturated condition of the as-precipitated salt.

B. Rate of Oxide Film Formation and Dissolution

Mrowec and Przybylski [30] have measured parabolic rate constants for the oxidation of cobalt to CoO at various oxygen partial pressures and temperatures. Under the conditions of our modeling calculations, a reasonable value of the parabolic rate constant for Co oxidation to CoO is 10^{-9} $g^2/cm^4 \cdot s$. Birks and Meir [31] give an order of magnitude estimate of the parabolic rate constant for chromium oxidation to Cr_2O_3 as 10^{-11} $g^2/cm^4 \cdot s$. Clearly formation of Cr_2O_3 is the slower of the oxidation processes, providing further justification for assuming, to a first approximation, that it is the chemical behavior of this component which has the largest effect on superalloy corrosion rates. Fig. 8 shows a hypothetical growth curve for Cr_2O_3 film on pure Cr calculated using the above rate constant. The requirement for steady state is that the growth rate of the film is equal to the rate of chemical solution in the molten salt precipitate. Fig. 9 shows a plot of steady state mass removal rate vs. film thickness for the hypothetical case of a perfectly adherent film of Cr_2O_3 on chromium. It is apparent that to remove material at a reasonable rate of a few $mg/cm^2/h$ would require very thin oxide films of submicron thickness.

VII. CHEMICAL CORROSION MODEL

A. Preliminary Test of Model

By assuming submicron thick steady state Cr_2O_3 films and combining information on rate of oxide film removal from Fig. 9 with estimates of salt deposition rates from Table 5, it is clearly seen that, allowing for the effect of Cr dilution in the superalloy and assuming 50 mole % solution of the oxide in the salt phase, corrosion rates in the range 0.1 to 50 $mg/cm^2/h$ are readily

attainable. These are in reasonable agreement with the range of test-rig data of ref. [32].

B. Discussion and future Plans

It appears that our integrated chemical corrosion model, though an over-simplification at this stage of development, has sufficient flexibility to produce a large range of reasonable corrosion rates, based solely upon the equilibrium solution chemistry. It therefore appears advisable to proceed in this direction, by attempting to make the model fully quantitative. This will require additional phase equilibrium and solubility data for the system $Na_2V_2O_6$-Na_2SO_4-V_2O_5-CoO-Cr_2O_3. Also it will be necessary to modify the CFBL program to calculate simultaneously precipitation rates of more than one salt species.

There are a number of features observed experimentally which future modeling efforts should address. The formation of a sulfide layer is not consistent with the equilibrium chemistry presented here, and may require application of the principles of local equilibrium and mass transport at the metal interface. Also, an intergranular component seems to be prevalent in high temperature hot corrosion. It is possible that an intergranular chemical solution approach could be useful here as well and could be related directly to the processes of physical removal of metal from the walls.

VIII. ACKNOWLEDGEMENTS

The authors wish to express their appreciation to Dr. Dasara Rathnamma for her encouragement in this project. Discussion with Drs. Robert Jones and Kurt

Stern of NRL have been helpful and Dr. Gokoglu has offered advice on the use of his computer code. Dr. John Hastie of NBS has offered valuable suggestions for improvement of this report.

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X. TABLES

Table 1. Impurity Concentration in Navy Test Fuels

Fuel (Composition)	Na (ppm. wt)	S (wt%)	V (ppm. wt.)
Base Fuel ($CH_{2.0}$)	1.0	0.07	0.5
GT 10 ($CH_{1.8}$)	1.0	1.0	0.5
GT 12 ($CH_{1.8}$)	2.0	2.0	2.0

Table 2. Matrix of Fuel Impurity Concentrations Used in Concentrations Used in Modeling

	Na (ppm. wt.)	S (wt. %)	V (ppm. wt.)
(1)	0.1	0.01	0.1
(2)	1.0	0.1	1.0
(3)	10.0	1.0	10.0

TABLE 3. Species Considered by CEC

L 5/66	AR	J 3/78	C	J12/67	CH	J12/72	CH2	J 3/61	CH2O
L 5/80	CH2O2	J 6/69	CH3	BUR 84	CH2OH	L 6/80	CH3O	L 5/84	CH4
L 4/80	CH3OH	J 6/69	CN	J12/70	CN2	J 6/66	CNN	J 9/65	CO
J 3/61	COS	J 9/65	CO2	J12/76	CS	J12/76	CS2	J12/69	C2
J 3/67	C2H	J 3/61	C2H2	BUR 84	C2H3	L 4/80	C2H4	L 5/80	C2H4O2
L 5/80	C2H4O4	A10/83	C2H5	L 5/84	C2H6	BUR 84	CH3N2CH3	BUR 84	C2H5OH
BUR 84	CH3OCH3	J 3/67	C2N	J 3/61	C2N2	J 9/66	C2O	J12/69	C3
L11/80	C3H6O	BUR 84	N-C3H7	BUR 84	I-C3H7	L 4/80	C3H8	L 1/84	1-C3H7OH
J 6/68	C3O2	J12/69	C4	L 5/80	C4H8O4	L 4/80	N-C4H10	L 5/80	I-C4H10
J 3/61	C4N2	J12/69	C5	L 1/84	C6H5	L 4/84	C6H5O	L 1/84	C6H6
L 4/84	C6H5OH	BUR 84	C7H8	P12/52	C8H16	P 4/81	N-C8H18	P10/74	I-C8H18
L 1/84	O-C12H9	L 4/84	C12H10	J 3/77	H	L12/69	HCN	J12/70	HCO
J12/70	HNCO	J 3/63	HNO	J 6/63	HNO2	J 6/63	HNO3	J 9/78	HO2
J 3/77	H2	J12/65	H2N2	J 3/79	H2O	L 6/80	H2O2	J 6/77	H2S
J 9/77	H2SO4	J 3/77	N	J12/70	NCO	J 6/77	NH	J 6/77	NH2
J 6/77	NH3	J 6/63	NO	J 9/64	NO2	J12/64	NO3	J 3/77	N2
J12/65	N2H4	J12/64	N2O	J 9/64	N2O4	J12/64	N2O5	J12/70	N3
J 6/62	NA	J3/66	NACN	J 3/63	NAH	J12/67	NAO	J12/70	NAOH
J 6/62	NA2	J3/66	NA2C2N2	K10/74	NA2O	J12/70	NA2O2H2	J 6/78	NA2SO4
J 3/77	O	J 6/77	OH	J 3/77	O2	J 6/61	O3	J 9/77	S
J 6/77	SH	J 6/61	SN	J 6/77	SO	J 6/61	SO2	J 9/65	SO3
J 9/77	S2	J 9/65	S2O	J6/64	S8	J 6/73	V	J12/73	VN
J12/73	VO	J12/73	VO2	J 3/78	C(GR)	P10/80	C7H8(L)	P10/80	C8H18(L)
L 3/81	H2O(S)	J 3/79	H2O(L)	J 9/77	H2SO4(L)	J12/73	VN(S)	BAR 77	N2H8SO4(S)
J 6/62	NA(S)	J 6/62	NA(L)	J 3/66	NACN(S)	J 3/66	NACN(L)	J12/70	NAOH(A)
J12/70	NAOH(L)	J 6/63	NAO2(S)	J 3/66	NA2CO3(1)	J 3/66	NA2CO3(2)	J 3/66	NA2CO3(L)
J 6/68	NA2O(C)	J 6/68	NA2O(A)	J 6/68	NA2O(L)	J 6/68	NA2O2(A)	J 6/68	NA2O2(B)
J 3/78	NA2S(1)	J 3/78	NA2S(2)	J 3/78	NA2S(L)	BAR 77	NA2SO3(S)	BAR 77	NA2SO3(L)
J 6/78	NA2SO4(IV)	J 6/78	NA2SO4(I)	J 6/78	NA2SO4(L)	J 9/77	S(S)	J 9/77	S(L)
J 6/73	V(S)	J 6/73	V(L)	KDA 84	NAV3O8(S)	KDA 84	NA2V12O31(S)	KDA 84	NA2V12O31(L)
BAR 73	NA2V2O6(S)	BAR 73	NA2V2O6(L)	BAR 73	NA4V2O7(S)	BAR 73	NA6V2O8(S)	BAR 73	NA6V2O8(L)
BAR 73	VO(S)	BAR 73	VO(L)	BAR 73	VO2(S)	BAR 73	VO2(S)	BAR 73	VO2(L)
BAR 73	V2O3(S)	BAR 73	V2O3(L)	BAR 73	V2O5(S)	BAR 73	V2O5(L)		

TABLE 4. Cofficients for V_4O_{10}
(CEC format)

```
Based on Semenov, et al [1970]
V4O10             SB1/87V   40  10    0    0G   300.000  5000.000          1
 0.45894528E+02 0.0             0.0             0.0            0.0          2
-0.36143218E+06-0.22261447E+03 0.45894528E+02 0.0            0.0          3
 3.0           -0.36143218E+06-0.22261447E+03                               4

Based on Polyakov [1946]
V4O10             PB1/87V   40  10    0    0G   300.000  5000.000          1
 0.45894528E+02 0.0             0.0             0.0            0.0          2
-0.35802894E+06-0.21333830E+03 0.45894528E+02 0.0            0.0          3
 3.0           -0.35802894E+06-0.21333830E+03                               4
```

Table 5. CFBL Salt Deposition Rates

T = 1172 K P = 1 atm

Composition Code	Liquid Mole Fractions Na_2SO_4	$Na_2V_2O_6$	V_2O_5	Salt Deposition Rate ($mg/h/cm^2$)
131	0.01433	0.87555	0.11011	0.1611
231	0.33446	0.6618	0.0036	0.0451
331	0.99378	0.0061	0.0000	0.3542
132	0.0005	0.20862	0.79091	8.574
232	0.15898	0.83149	0.0094	0.1804
332	0.93993	0.059908	0.0001	0.3787
133	0.0000	0.02181	0.97815	105.304
233	0.0005	0.21967	0.77982	84.1427
333	0.48135	0.51653	0.0019	0.8106

TABLE 6. CFBL THEORY FOR SODIUM SULFATE DEPOSITION RATE

CASE NO. 8701 131 0.1 ppm Na, 1%S, 0.1 ppm V V1R0P1HT

- - INPUT PARAMETERS - - (ALL GAS PROPERTIES PERTAIN TO TJ,PJ)

RUN = 19 TYPE = 0
TO (K) = 1806.000 PO (ATM) = 1.068000
TW (K) = 1172.000 PJ (ATM) = 1.000000
Fuel/Air Mass Ratio (F) = 0.045380
Air Flow Rate (WA, G/SEC) = 2.94000
Dia. Cyl. Target (DIAW, CM) = 0.31800
Length (hgt) Target (LW, CM) = 3.81000
Dia. Jet Nozzle (DJ, CM) = 6.03300
Observed Deposition rate (WOBS, MG/HR) = 0.0045
FSORET? = T

OPTIONAL PARAMETERS
Nozzle Discharge Coef (DC) = 1.000000
SHAPE = 0.0000 DIV = 0.0000
TURBULANCE
TURB = 0.0000
TURIN = 0.0000 PERCENT
TURL (CM) = 0.00000

I=1=NAOH , I=2=NA , I=3=NA2SO4 , I=6=NACL

I	D(I)	NU(I)	SC(I)	X(I),	J X(I),W	TAU(I)	F(SORET),I	M(I)
1	0.27773E+01	0.39893E+01	0.10853E+01	0.50180E-08	0.13280E-08	0.45016E-01	1.02268	0.89010E-03
2	0.35112E+01	0.36321E+01	0.85843E+00	0.41340E-09	0.00000E+00	-0.15846E-01	0.99210	0.10953E-03
3	0.17005E+01	0.48542E+01	0.17725E+01	0.14160E-16	0.95190E-09	0.17019E+00	1.08751	-0.29915E-03
6	0.23382E+01	0.42736E+01	0.12891E+01	0.00000E+00	0.00000E+00	0.92532E-01	1.04698	0.00000E+00

YNAJ	YNAW	YSJ	YSW
0.543140E-08	0.323180E-08	0.394772E-03	0.394881E-03

Average Molec. Wt.= 28.81275
Turbulance factor = 1.00000
Re(EFF) = 57.533
Total Na mass flux to surface (SUM, G/CM**2/SEC) = 1.65482E-11
Total S mass flux to surface (SMS, G/CM**2/SEC) = 3.92336E-07
Na-to-S molar flux ratio at the surface = 0.0001

PREDICTED NA2SO4 DEPOSITION RATE (MG/HR) = 7.00474E-04
ERROR (%) = -8.443E+01

GM = 1.26949
TJ (K) = 1780.95
PR = 0.690190
MOLE FRACTIONS
X(N2) = 0.755099
X(O2) = 0.065770
X(H2O) = 0.089565
X(CO2) = 0.089565

RHOJ(G/CM**3)	UJ(CM/S)	ETAMIX(POISE)	LAMIX(CAL/CM/K/S)	CMIX(CAL/G/S)
0.197159E-03	0.545317E+03	0.594261E-03	0.279215E-03	0.324288E+00

XI. ILLUSTRATIONS

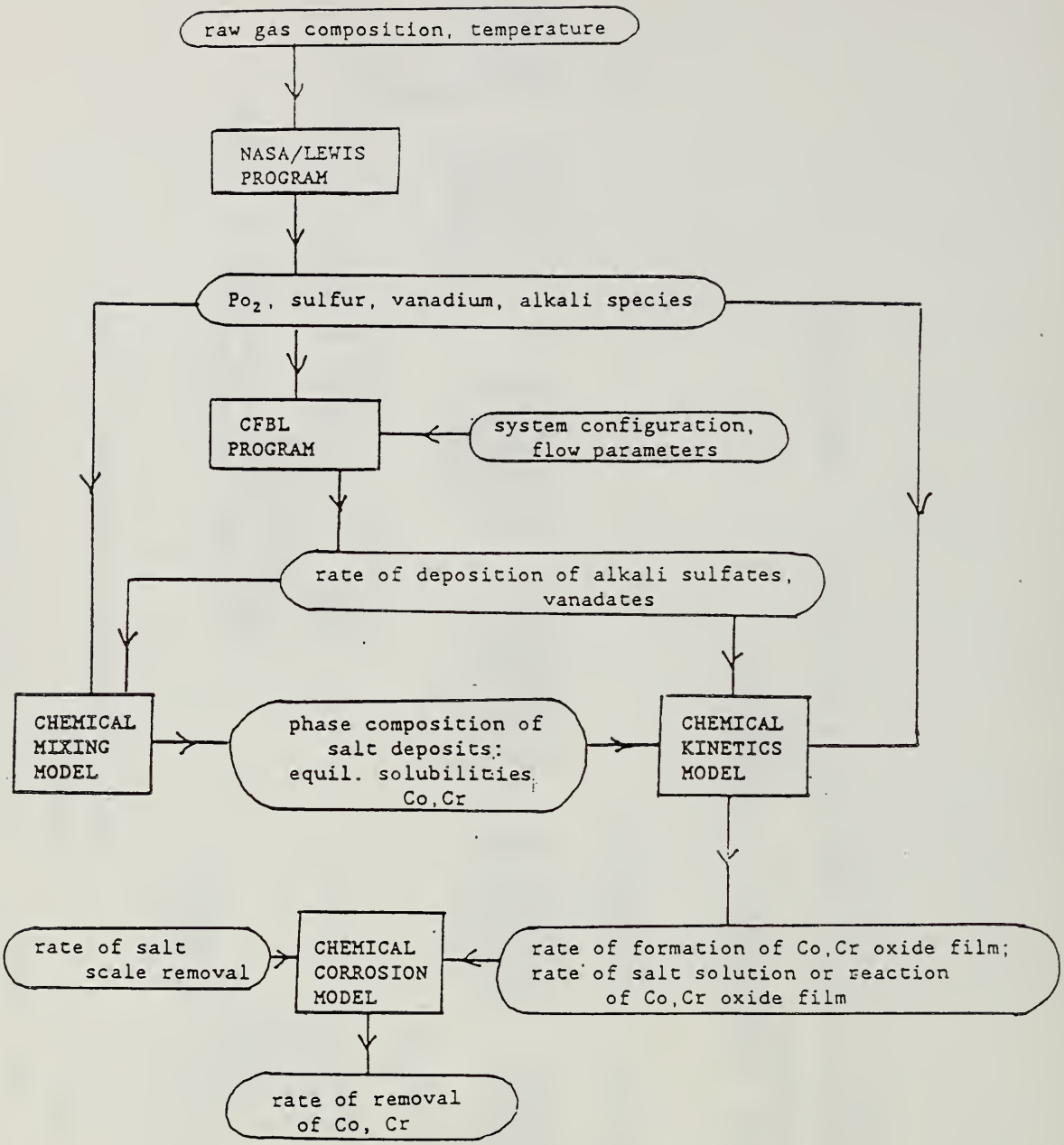

raw gas composition, temperature
NASA/LEWIS PROGRAM
Po_2, sulfur, vanadium, alkali species
CFBL PROGRAM
system configuration, flow parameters
rate of deposition of alkali sulfates, vanadates
CHEMICAL MIXING MODEL
phase composition of salt deposits: equil. solubilities Co,Cr
CHEMICAL KINETICS MODEL
rate of salt scale removal
CHEMICAL CORROSION MODEL
rate of formation of Co,Cr oxide film; rate of salt solution or reaction of Co,Cr oxide film
rate of removal of Co, Cr

Figure 1. Flow chart of molten salt/superalloy corrosion model.

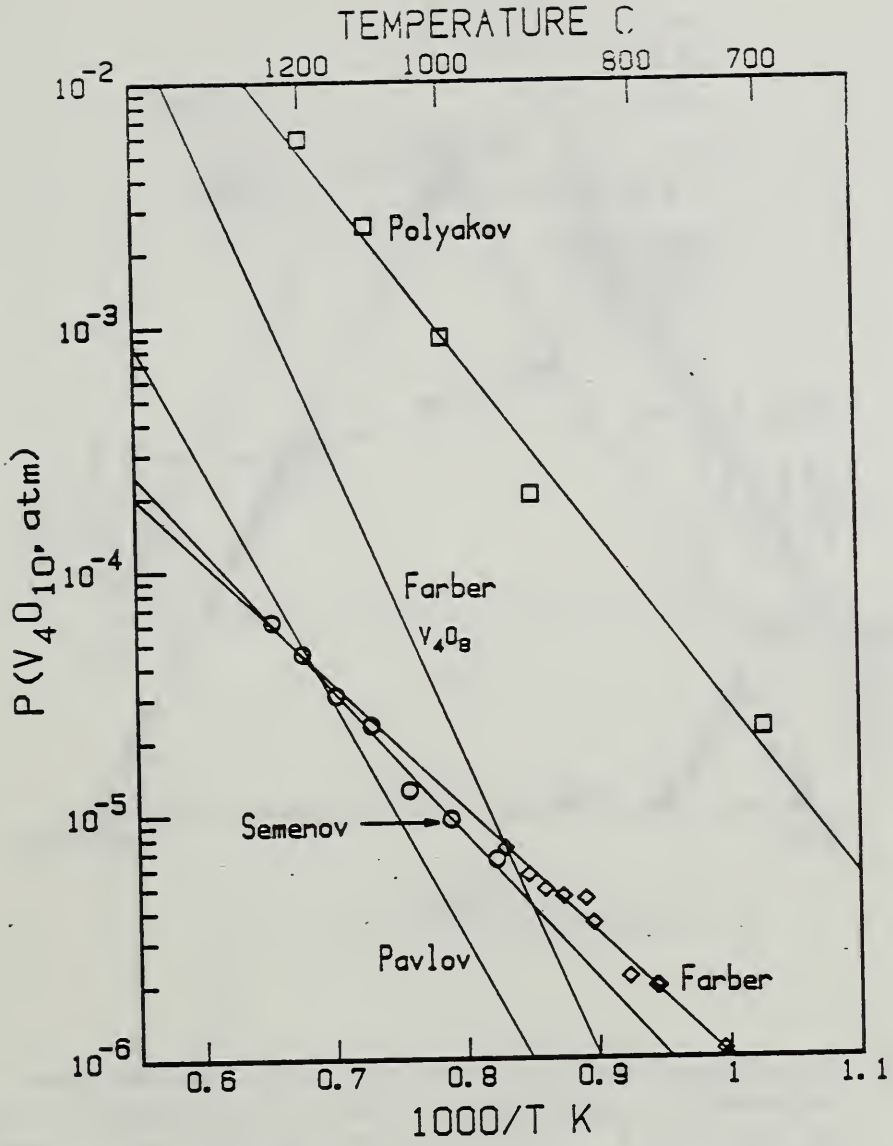


Figure 2. Partial pressures of species in the system V-O. Data from Polyakov [18], Semenov et al. [19], and Farber et al. [20]. Data and curves are for $2V_2O_5(c) = V_4O_{10}(g)$, except "Farber V_4O_8", which is presumably a decomposition process. Only the Farber data are species specific measurements.

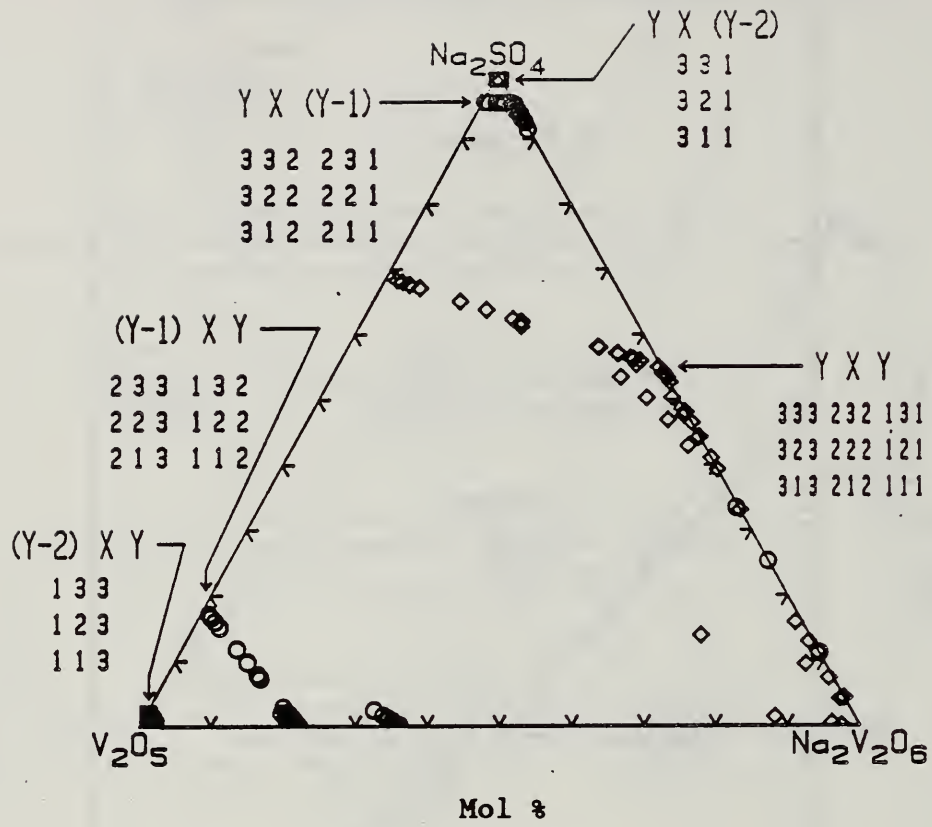
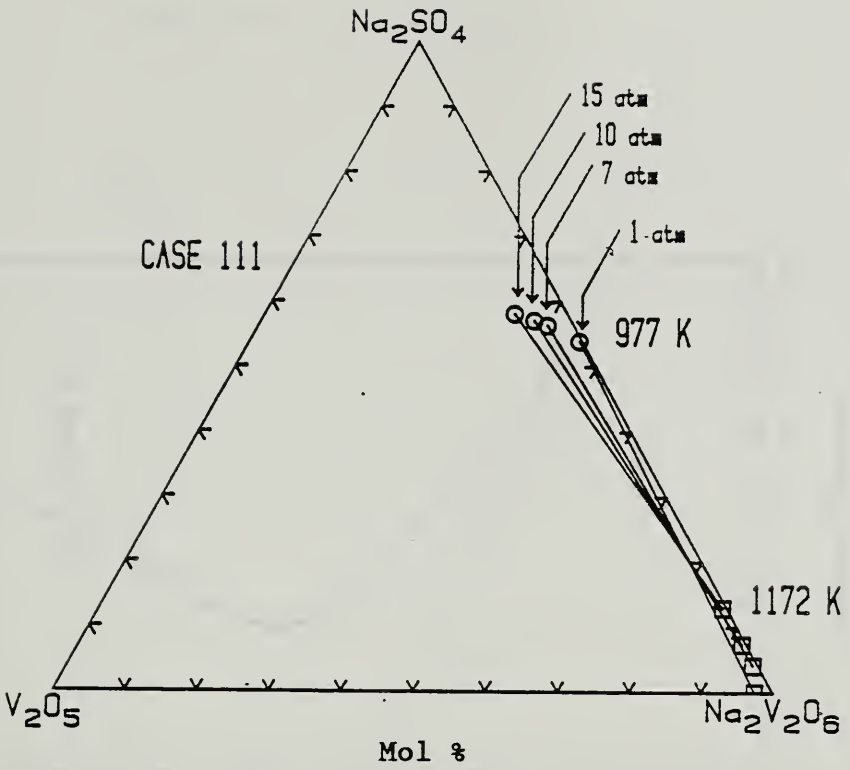
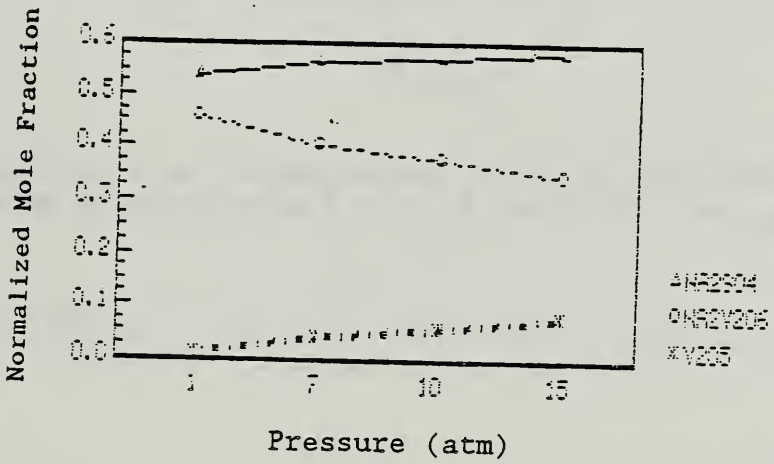


Figure 3. Calculated equilibrium molten salt compositions produced by combustion of fuels with impurity levels as in Table 2. Calculations completed at 977 and 1172 K and at 1, 5, 10 and 15 atm (see Appendix A).



A.



B.

Figure 4. Effect of pressure and temperature on molten salt composition produced from (111) fuel (0.1 ppm Na, 0.01 wt% S, 0.1 ppm V). A) ternary plot. B) effect of pressure at constant temperature (977 K).

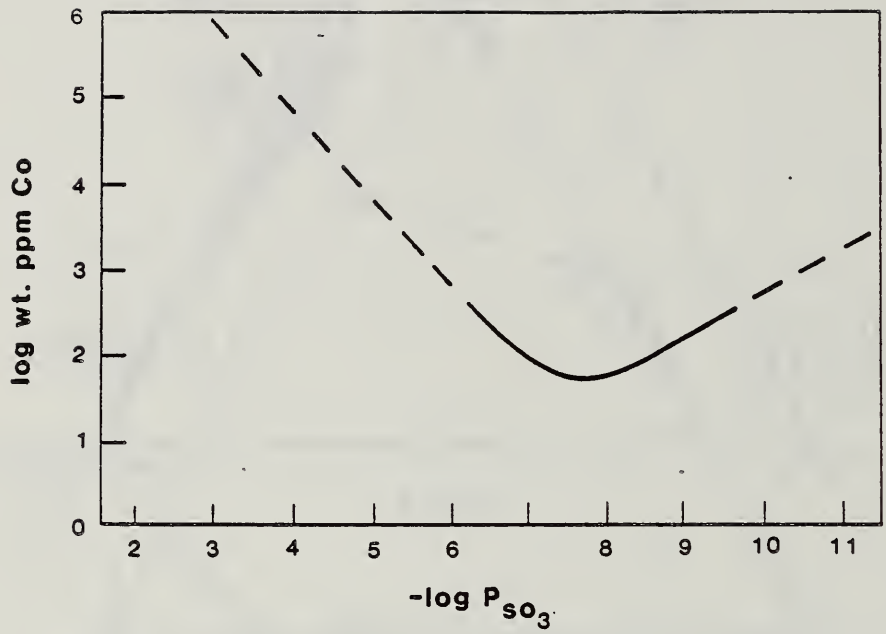


Figure 5. Solubility of CoO in molten Na_2SO_4 as a function of P_{SO_3} at 1200 K and P_{O_2} = 0.2 atm (modified after ref [27]).

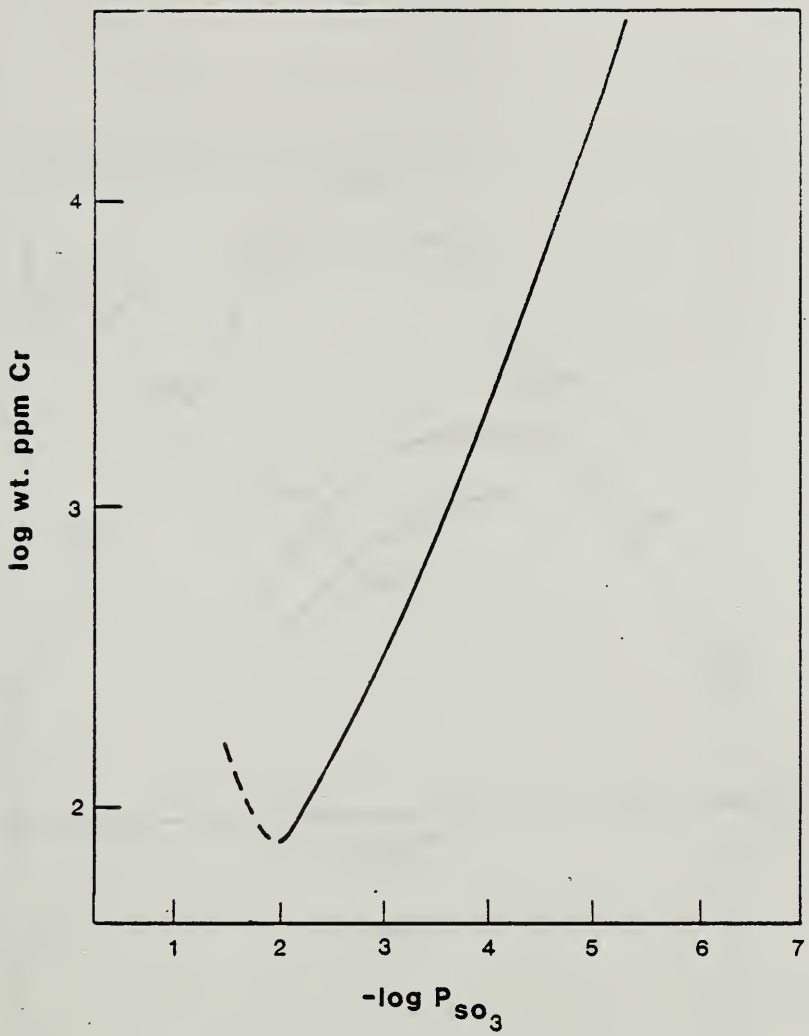


Figure 6. Solubility of Cr_2O_3 in molten Na_2SO_4 at 1200 K and $P_{O_2} \sim 7 \times 10^{-2}$ atm. (modified after ref [28]).

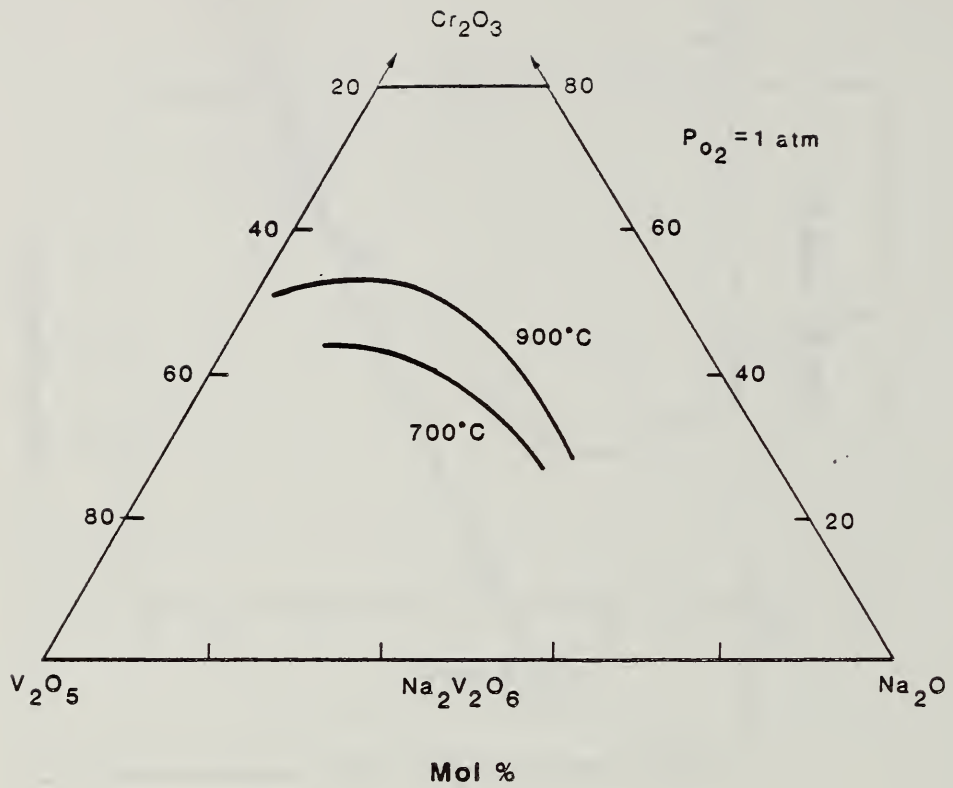


Figure 7. Solubility isotherms for Cr_2O_3 in sodium vanadate melts at 700° and 900 °C (modified after ref [29]).

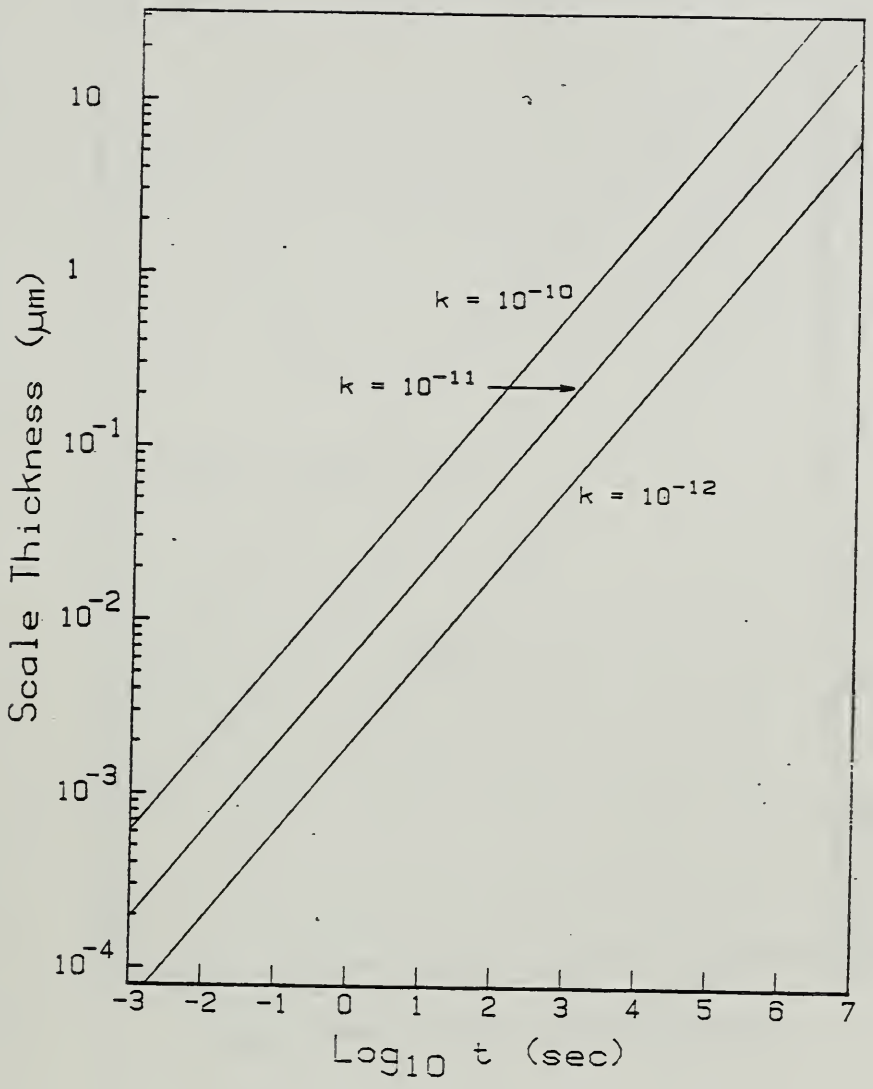


Figure 8. Calculated growth curves of Cr_2O_3 film on Cr metal for various parabolic rate constants.

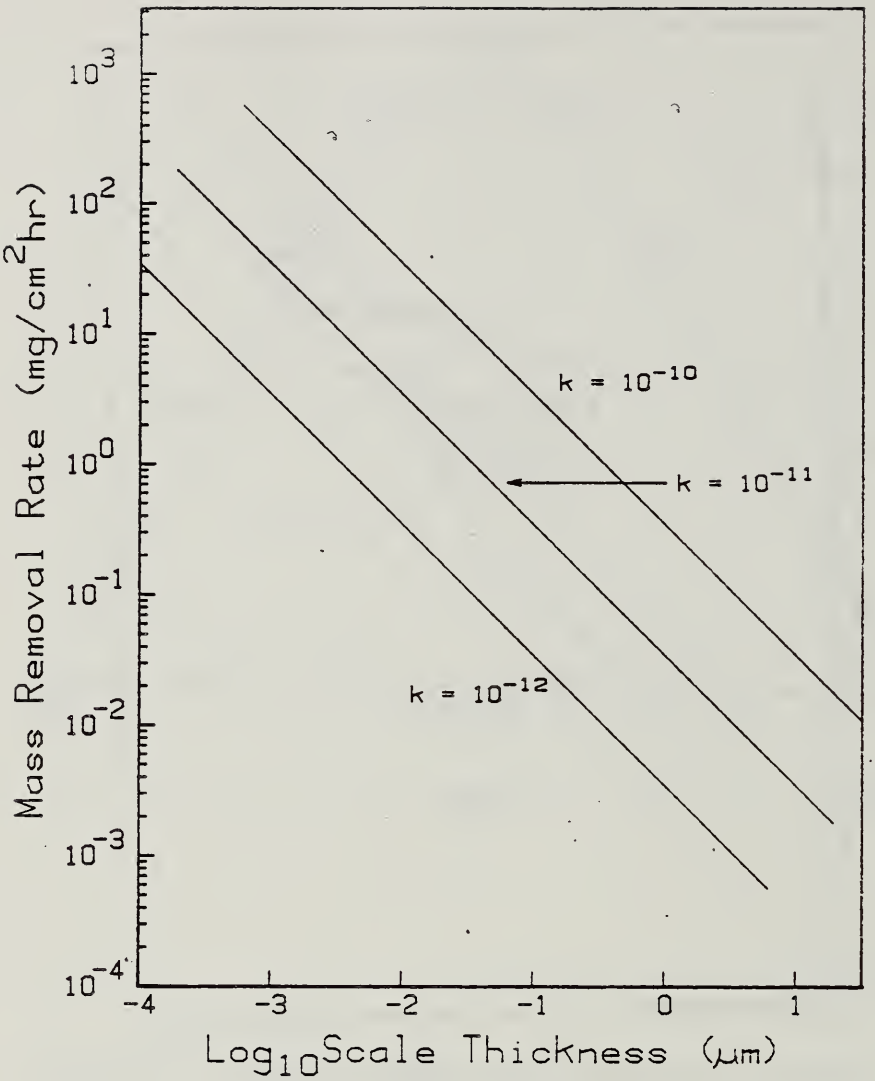


Figure 9. Film thickness vs. steady state mass removal rate for Cr_2O_3 film on Cr for the three different rate constants of Fig. 8.

XII. APPENDICES

Appendix A. CEC calculations of gas/condensed phase equilibria for fuels with various impurity levels (see Table 2).

SOLN 1 GASES

SOLN 2 V2O5(L) V2O3(L) V2O4(L) VCL4(L)
SOLN 2 NA2SO3(L) NA2SO4(L) NAOH(L)
SOLN 2 NA2O(L) NA2V2O6(S) NA4V2O7(S) NA6V2O8(S)

CASE NO. 8701 111 0.01%SULFUR, 0.1 NA, 0.1 V PPM TIME = 1.384 SEC

P, ATM	1.0000	1.0000	5.0000	5.0000	7.0000	7.0000	10.000	10.000	15.000	15.000
T, DEG K	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0
SOLUTION 1										
AR	8.8005-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3
CO	3.0980-9	9.536-12	1.3860-9	4.265-12	1.1710-9	3.604-12	9.798-10	3.016-12	8.000-10	2.462-12
CO2	9.0898-2	9.0898-2	9.0898-2	9.0898-2	9.0898-2	9.0898-2	9.0898-2	9.0898-2	9.0898-2	9.0898-2
H	5.874-12	4.834-15	1.757-12	1.446-15	1.365-12	1.123-15	1.045-12	8.596-16	7.707-13	6.342-16
HNO	1.515-12	1.651-14	2.265-12	2.469-14	2.464-12	2.686-14	2.694-12	2.936-14	2.981-12	3.250-14
HNO2	4.1197-9	1.6058-9	1.3775-8	5.3694-9	1.7729-8	6.9107-9	2.3166-8	9.0302-9	3.1400-8	1.2239-8
HNO3	1.205-11	1.509-11	9.011-11	1.128-10	1.372-10	1.718-10	2.143-10	2.683-10	3.358-10	4.454-10
HO2	1.1950-8	9.702-10	1.7870-8	1.4510-9	1.9440-8	1.5780-9	2.1250-8	1.7250-9	2.3520-8	1.9090-9
H2	2.6140-9	1.618-11	1.1690-9	7.235-12	9.882-10	6.114-12	8.268-10	5.116-12	6.751-10	4.177-12
H2O	9.6947-2	9.6948-2	9.6947-2	9.6948-2	9.6947-2	9.6948-2	9.6947-2	9.6948-2	9.6948-2	9.6948-2
H2O2	4.817-10	5.487-11	1.0770-9	1.227-10	1.2750-9	1.452-10	1.5230-9	1.735-10	1.8660-9	2.125-10
H2SO4	2.731-11	8.255-10	2.786-10	6.2600-9	4.485-10	9.3690-9	7.395-10	1.4250-8	1.2970-9	2.2750-8
NO	9.4443-5	1.4817-5	9.4442-5	1.4816-5	9.4442-5	1.4816-5	9.4441-5	1.4816-5	9.4441-5	1.4816-5
NO2	1.0011-6	5.1936-7	2.2385-6	1.1613-6	2.6487-6	1.3741-6	3.1657-6	1.6423-6	3.8772-6	2.0114-6
NO3	1.255-13	2.774-14	6.274-13	1.387-13	8.784-13	1.942-13	1.255-12	2.774-13	1.882-12	4.162-13
N2	7.3699-1	7.3703-1	7.3699-1	7.3703-1	7.3699-1	7.3703-1	7.3699-1	7.3703-1	7.3699-1	7.3703-1
N2O	5.5982-9	1.0091-9	1.2518-8	2.2563-9	1.4811-8	2.6697-9	1.7703-8	3.1909-9	2.1681-8	3.9081-9
NAOH	2.9560-9	1.071-11	2.3730-9	2.504-11	2.1130-9	1.228-12	1.8330-9	8.382-13	1.4970-9	5.466-13
NA2SO4	4.697-11	6.046-11	3.088-10	2.5090-9	3.942-10	9.023-12	4.890-10	6.398-12	5.722-10	4.342-12
O	3.4940-9	1.966-11	1.5630-9	8.794-12	1.3210-9	7.432-12	1.1050-9	6.218-12	9.022-10	5.077-12
OH	1.5471-6	5.5772-8	1.0346-6	3.7297-8	9.5112-7	3.4288-8	8.6998-7	3.1363-8	7.8611-7	2.8340-8
O2	6.6260-2	6.6300-2	6.6259-2	6.6299-2	6.6259-2	6.6299-2	6.6258-2	6.6299-2	6.6257-2	6.6298-2
O3	1.882-12	9.957-14	4.208-12	2.226-13	4.979-12	2.634-13	5.951-12	3.148-13	7.288-12	3.856-13
SO2	3.6779-6	2.4636-6	3.3559-6	1.6711-6	3.2611-6	1.5097-6	3.1489-6	1.3450-6	3.0065-6	1.1684-6
SO3	3.0907-7	1.5212-6	6.3059-7	2.3072-6	7.2505-7	2.4664-6	8.3679-7	2.6262-6	9.7849-7	2.7942-6
M, MOL WT	28.868	28.868	28.868	28.868	28.868	28.868	28.868	28.868	28.868	28.868
PHASE FRACTION	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0
SOLUTION 2										
NAOH(L)	2.4494-6	4.6960-7	0.000000	0.000000	1.2256-5	3.7695-7	1.5188-5	3.6767-7	1.8607-5	3.5965-7
NA2SO3(S)	0.000 0	4.920-12	0.000 0	0.000 0	0.000 0	1.943-12	0.000 0	1.647-12	0.000 0	1.369-12
NA2SO3(L)	2.559-12	0.000 0	0.000 0	0.000 0	5.682-11	0.000 0	8.425-11	0.000 0	1.207-10	0.000 0
NA2SO4(I)	0.000000	5.3928-1	0.000000	0.000000	0.000000	5.6338-1	0.000000	5.7070-1	0.000000	5.8101-1
NA2SO4(L)	7.0718-4	0.000000	0.000000	0.000000	4.1540-2	0.000000	7.3616-2	0.000000	1.2921-1	0.000000
NA2V2O6(L)	9.7433-1	4.5694-1	0.000000	0.000000	9.5165-1	4.0067-1	9.2007-1	3.7833-1	8.6485-1	3.4593-1
NA4V2O7(S)	5.0912-5	1.1436-5	0.000000	0.000000	0.000000	9.2305-7	1.8485-4	5.8043-7	1.7387-4	3.3855-7
NA6V2O8(S)	1.296-11	0.000 0	0.000 0	0.000 0	1.619-10	0.000 0	1.809-10	0.000 0	1.702-10	0.000 0
V2O3(S)	7.7880-8	5.627-11	0.000 0	0.000 0	3.0380-9	7.657-11	1.9130-9	7.600-11	1.1980-9	7.263-11
V2O5(L)	2.4909-2	3.7736-3	0.000000	0.000000	6.8014-3	3.5947-2	6.1176-3	5.0970-2	5.7467-3	7.3060-2
M, MOL WT	242.25	188.72	0.0000	0.0000	239.21	184.27	235.99	182.59	230.35	180.17
PHASE FRACTION	1.2309-9	2.6697-9	0.000000	0.000000	1.2833-9	2.8171-9	1.3277-9	2.8651-9	1.4125-9	2.9356-9
PURE SPECIES PHASE FRACTIONS (IF ANY)										
NA2V12O31(L)	0.000 0	0.000 0	0.000 0	2.050-10	0.000 0	0.000 0	0.000 0	0.000 0	0.000 0	0.000 0

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-11 FOR ALL ASSIGNED CONDITI

SOLUTION 1

C	CH	CH2	CH2O	CH2O2	CH3	CH2OH	CH3O	CH4	CH
CN	CN2	CNN	COS	CS	CS2	C2	C2H	C2H2	C2
C2H4	C2HAO2	C2H4O4	C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3	C2N	C2
C2O	C3	C3H6O	N-C3H7	I-C3H7	C3H8	1-C3H7OH	C3O2	C4	C4
N-C4H10	I-C4H10	C4N2	C5	C6H5	C6H5O	C6H6	C6H5OH	C7H8	C8
N-C8H18	I-C8H18	O-C12H9	C12H10	HCN	HCO	HNCO	H2N2	H2S	N
NCO	NH	NH2	NH3	N2H4	N2O4	N2O5	N3	NA	NA
NAH	NAO	NA2	NA2C2N2	NA2O	NA2O2H2	S	SH	SN	SO
S2	S2O	S8	V	VN	VO	VO2			
SOLUTION 2									
NAOH(A)	NA2O(C)	NA2O(A)	NA2O(L)	NA2SO4(IV)	NA2V2O6(S)	NA6V2O8(L)	V2O3(L)	V2O5(S)	
PURE SPECIES									
C(GR)	C7H8(L)	C8H18(L)	H2O(S)	H2O(L)	H2SO4(L)	VN(S)	N2H6SO4(S)	NA(S)	NA
NACN(S)	NACN(L)	NAO2(S)	NA2CO3(1)	NA2CO3(2)	NA2CO3(L)	NA2O2(A)	NA2O2(B)	NA2S(1)	NA
NA2S(L)	S(S)	S(L)	V(S)	V(L)	NAV3O8(S)	NA2V12O31(S)	VO(S)	VO(L)	VO
VO2(S)	VO2(L)								

CASE NO. 8701 211 0.01%SULFUR, 1.0 NA, 0.1 V PPM

P, ATM	1.0000
T, DEG K	1172.0
SOLUTION 1	
AR	8.8005-3
CO	3.0982-9
CO2	9.0898-2
H	5.874-12
HNO	1.515-12
HNO2	4.1197-9
HNO3	1.205-11
HO2	1.1950-8
H2	2.6144-9
H2O	9.6947-2
H2O2	4.817-10
H2SO4	2.726-11
NO	9.4443-5
NO2	1.0011-6
N2	7.3699-1
N2O	5.5982-9
NA	4.788-12
NAOH	3.7017-8
NA2SO4	7.3506-9
O	3.4941-9
OH	1.5471-6
O2	6.6260-2
O3	1.882-12
SO2	3.6710-6
SO3	3.0849-7
M, MOL WT	28.868
PHASE FRACTION	1.0000 0
SOLUTION 2	
NAOH(L)	3.0668-5
NA2O(C)	1.934-12
NA2SO3(L)	4.005-10
NA2SO4(L)	1.1066-1
NA2V2O6(L)	8.8194-1
NA4V2O7(S)	7.2248-3
NA6V2O8(S)	2.8827-7
V2O3(S)	4.497-10
V2O5(L)	1.4382-4
M, MOL WT	233.02
PHASE FRACTION	1.3831-9

PURE SPECIES PHASE FRACTIONS (IF ANY)

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-11 FOR ALL ASSIGNED CONDITI

SOLUTION 1

C	CH	CH2	CH2O	CH2O2	CH3	CH2OH	CH3O	CH4	CH
CN	CN2	CNN	COS	CS	CS2	C2	C2H	C2H2	C2
C2H4	C2H4O2	C2H4O4	C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3	C2N	C2
C2O	C3	C3H6O	N-C3H7	I-C3H7	C3H8	1-C3H7OH	C3O2	C4	C4
N-C4H10	I-C4H10	C4N2	C5	C6H5	C6H5O	C6H6	C6H5OH	C7H8	C8
N-C8H18	I-C8H18	O-C12H9	C12H10	HCN	HCO	HNCO	H2N2	H2S	N
NCO	NH	NH2	NH3	NO3	N2H4	N2O4	N2O5	N3	NA
NAH	NAO	NA2	NA2C2N2	NA2O	NA2O2H2	S	SH	SN	SO
S2	S2O	S8	V	VN	VO	VO2			

SOLUTION 2

NAOH(A)	NA2O(A)	NA2O(L)	NA2SO3(S)	NA2SO4(IV)	NA2SO4(I)	NA2V2O6(S)	NA6V2O8(L)	V2O3(L)	V2

PURE SPECIES

C(GR)	C7H8(L)	C8H18(L)	H2O(S)	H2O(L)	H2SO4(L)	VN(S)	N2H6SO4(S)	NA(S)	NA
NACN(S)	NACN(L)	NAO2(S)	NA2CO3(1)	NA2CO3(2)	NA2CO3(L)	NA2O2(A)	NA2O2(B)	NA2S(1)	NA
NA2S(L)	S(S)	S(L)	V(S)	V(L)	NAV3O8(S)	NA2V12O31(S)	NA2V12O31(L)	VO(S)	VO
VO2(S)	VO2(S)	VO2(L)							

CASE NO. 8701 311 0.01%SULFUR, 10 NA, 0.1 V PPM TIME = 0.520 SEC

P, ATM	1.0000	1.0000	5.0000	5.0000	7.0000	7.0000	10.000	10.000	15.000	15.000
T, DEG K	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0
SOLUTION 1										
AR	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3
CO	3.0980-9	9.536-12	1.3860-9	4.265-12	1.1710-9	3.604-12	9.797-10	3.015-12	8.000-10	2.462-12
CO2	9.0897-2	9.0897-2	9.0897-2	9.0897-2	9.0897-2	9.0897-2	9.0897-2	9.0897-2	9.0897-2	9.0897-2
H	5.874-12	4.834-15	1.757-12	1.446-15	1.365-12	1.123-15	1.045-12	8.596-16	7.707-13	6.342-16
HNO	1.515-12	1.651-14	2.265-12	2.469-14	2.464-12	2.686-14	2.694-12	2.936-14	2.981-12	3.250-14
HNO2	4.1198-9	1.6059-9	1.3775-8	5.3695-9	1.7729-8	6.9107-9	2.3167-8	9.0303-9	3.1400-8	1.2240-8
HNO3	1.205-11	1.509-11	9.011-11	1.128-10	1.372-10	1.718-10	2.143-10	2.683-10	3.558-10	4.454-10
HO2	1.1950-8	9.702-10	1.7870-8	1.4510-9	1.9440-8	1.5780-9	2.1250-8	1.7250-9	2.3520-8	1.9090-9
H2	2.6140-9	1.618-11	1.1690-9	7.234-12	9.881-10	6.114-12	8.267-10	5.116-12	6.750-10	4.177-12
H2O	9.6946-2	9.6947-2	9.6947-2	9.6947-2	9.6947-2	9.6947-2	9.6947-2	9.6947-2	9.6947-2	9.6947-2
H2O2	4.817-10	5.487-11	1.0770-9	1.227-10	1.2750-9	1.452-10	1.5230-9	1.735-10	1.8660-9	2.125-10
H2SO4	2.584-11	7.696-10	2.602-10	5.8380-9	4.186-10	8.7350-9	6.899-10	1.3290-8	1.2100-9	2.1210-8
NO	9.4444-5	1.4817-5	9.4443-5	1.4817-5	9.4442-5	1.4817-5	9.4442-5	1.4817-5	9.4441-5	1.4817-5
NO2	1.0011-6	5.1937-7	2.2386-6	1.1613-6	2.6487-6	1.3741-6	3.1658-6	1.6423-6	3.8772-6	2.0114-6
NO3	1.255-13	2.775-14	6.274-13	1.387-13	8.784-13	1.942-13	1.255-12	2.774-13	1.882-12	4.162-13
N2	7.3699-1	7.3703-1	7.3699-1	7.3703-1	7.3699-1	7.3704-1	7.3699-1	7.3704-1	7.3699-1	7.3704-1
N2O	5.5983-9	1.0091-9	1.2518-8	2.2564-9	1.4811-8	2.6698-9	1.7703-8	3.1910-9	2.1682-8	3.9081-9
NA	1.472-11	4.811-17	6.215-13	2.337-18	3.218-13	1.254-18	1.605-13	6.512-19	7.303-14	3.105-19
NAO	1.750-12	9.350-18	1.652-13	1.015-18	1.012-13	6.449-19	6.034-14	4.001-19	3.362-14	2.337-19
NAOH	1.1380-7	1.507-11	1.6070-8	2.446-12	1.0710-8	1.690-12	6.9780-9	1.147-12	4.3030-9	7.410-13
NA2SO4	6.5870-8	1.116-10	1.3220-8	2.232-11	9.4430-9	1.594-11	6.6110-9	1.116-11	4.4080-9	7.440-12
O	3.4940-9	1.966-11	1.5630-9	8.794-12	1.3210-9	7.432-12	1.1050-9	6.218-12	9.022-10	5.077-12
OH	1.5471-6	5.5773-8	1.0346-6	3.7297-8	9.5112-7	3.4288-8	8.6998-7	3.1363-8	7.8611-7	2.8340-8
O2	6.6261-2	6.6301-2	6.6260-2	6.6300-2	6.6260-2	6.6300-2	6.6259-2	6.6300-2	6.6258-2	6.6299-2
O3	1.882-12	9.957-14	4.208-12	2.226-13	4.979-12	2.634-13	5.951-12	3.149-13	7.288-12	3.856-13
SO2	3.4802-6	2.2968-6	3.1345-6	1.5583-6	3.0439-6	1.4075-6	2.9378-6	1.2539-6	2.8041-6	1.0893-6
SO3	2.9246-7	1.4182-6	5.8899-7	2.1515-6	6.7676-7	2.2994-6	7.8069-7	2.4484-6	9.1261-7	2.6051-6
M, MOL WT	28.868	28.868	28.868	28.868	28.868	28.868	28.868	28.868	28.868	28.868
PHASE FRACTION	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0
SOLUTION 2										
NAOH(L)	9.4291-5	6.6079-7	6.6555-5	5.3648-7	6.2094-5	5.1895-7	5.7815-5	5.0291-7	5.3476-5	4.8736-7
NA2O(C)	1.828-11	0.000 0	1.822-12	0.000 0	1.133-12	0.000 0	0.000 0	0.000 0	0.000 0	0.000 0
NA2SO3(S)	0.000 0	9.082-12	0.000 0	4.062-12	0.000 0	3.433-12	0.000 0	2.872-12	0.000 0	2.345-12
NA2SO3(L)	3.5890-9	0.000 0	1.6110-9	0.000 0	1.3610-9	0.000 0	1.1390-9	0.000 0	9.301-10	0.000 0
NA2SO4(I)	0.000000	9.9548-1	0.000000	9.9549-1	0.000000	9.9549-1	0.000000	9.9549-1	0.000000	9.9549-1
NA2SO4(L)	9.9169-1	0.000000	9.9504-1	0.000000	9.9517-1	0.000000	9.9526-1	0.000000	9.9532-1	0.000000
NA2V2O6(L)	7.6267-3	4.4959-3	4.8563-3	4.3743-3	4.7479-3	4.3084-3	4.6708-3	4.2087-3	4.6128-3	4.0460-3
NA4V2O7(S)	5.9058-4	2.2280-7	3.7472-5	2.8577-8	2.2777-5	1.8812-8	1.3598-5	1.2081-8	7.6593-6	7.2770-9
NA6V2O8(S)	2.2270-7	0.000 0	1.4080-9	0.000 0	5.322-10	0.000 0	1.928-10	0.000 0	6.194-11	0.000 0
V2O5(L)	1.3157-7	1.8752-5	8.4075-7	1.3839-4	1.3221-6	2.0395-4	2.1432-6	3.0306-4	3.7110-6	4.6497-4
M, MOL WT	142.90	142.50	142.53	142.49	142.52	142.48	142.51	142.48	142.50	142.47
PHASE FRACTION	1.4967-7	2.7243-7	2.5129-7	2.7256-7	2.5775-7	2.7258-7	2.6245-7	2.7261-7	2.6599-7	2.7266-7

PURE SPECIES PHASE FRACTIONS (IF ANY)

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-11 FOR ALL ASSIGNED CONDITI

SOLUTION 1

C	CH	CH2	CH2O	CH2O2	CH3	CH2OH	CH3O	CH4	CH
CN	CN2	CNN	COS	CS	CS2	C2	C2H	C2H2	C2
C2H4	C2H4O2	C2H4O4	C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3	C2N	C2
C2O	C3	C3H6O	N-C3H7	I-C3H7	C3H8	1-C3H7OH	C3O2	C4	C4
N-C4H10	I-C4H10	C4N2	C5	C6H5	C6H5O	C6H6	C6H5OH	C7H8	C8
N-C8H18	I-C8H18	O-C12H9	C12H10	HCN	HCO	HNCO	H2N2	H2S	N
NCO	NH	NH2	NH3	N2H4	N2O4	N2O5	NS	NACN	NA
NA2	NA2C2N2	NA2O	NA2O2H2	S	SH	SN	SO	S2	S2
S8	V	VN	VO	VO2					

SOLUTION 2

NAOH(A)	NA2O(A)	NA2O(L)	NA2SO4(IV)	NA2V2O6(S)	NA6V2O8(L)	V2O3(S)	V2O3(L)	V2O5(S)

PURE SPECIES

C(GR)	C7H8(L)	C8H18(L)	H2O(S)	H2O(L)	H2SO4(L)	VN(S)	N2H6SO4(S)	NA(S)	NA
NACN(S)	NACN(L)	NAO2(S)	NA2CO3(1)	NA2CO3(2)	NA2CO3(L)	NA2O2(A)	NA2O2(B)	NA2S(1)	NA
NA2S(L)	S(S)	S(L)	V(S)	V(L)	NAV3O8(S)	NAZV12O31(S)	NAZV12O31(L)	VO(S)	VO
VO2(S)	VO2(S)	VO2(L)							

CASE NO. 8701 112 0.01%SULFUR, 0.1 NA, 1.0 V PPM TIME = 0.512 SEC

P, ATM	1.0000	1.0000	5.0000	5.0000	7.0000	7.0000	10.000	10.000	15.000	15.000
T, DEG K	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0
SOLUTION 1										
AR	8.8005-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3
CO	3.0980-9	9.536-12	1.3860-9	4.265-12	1.1710-9	3.604-12	9.798-10	3.016-12	8.000-10	2.462-12
CO2	9.0898-2	9.0898-2	9.0898-2	9.0898-2	9.0898-2	9.0898-2	9.0898-2	9.0898-2	9.0898-2	9.0898-2
H	5.874-12	4.834-15	1.757-12	1.446-15	1.365-12	1.123-15	1.045-12	8.596-16	7.707-13	6.342-16
HNO	1.515-12	1.651-14	2.265-12	2.469-14	2.464-12	2.686-14	2.694-12	2.936-14	2.981-12	3.250-14
HNO2	4.1197-9	1.6058-9	1.3775-8	5.3694-9	1.7729-8	6.9107-9	2.3166-8	9.0302-9	3.1400-8	1.2239-8
HNO3	1.205-11	1.509-11	9.011-11	1.128-10	1.372-10	1.718-10	2.143-10	2.683-10	3.558-10	4.454-10
HO2	1.1950-8	9.702-10	1.7870-8	1.4510-9	1.9440-8	1.5780-9	2.1250-8	1.7250-9	2.3520-8	1.9090-9
H2	2.6140-9	1.618-11	1.1690-9	7.235-12	9.882-10	6.114-12	8.268-10	5.116-12	6.751-10	4.177-12
H2O	9.6947-2	9.6948-2	9.6947-2	9.6948-2	9.6947-2	9.6948-2	9.6947-2	9.6948-2	9.6947-2	9.6948-2
H2O2	4.817-10	5.487-11	1.0770-9	1.227-10	1.2750-9	1.452-10	1.5230-9	1.735-10	1.8660-9	2.125-10
H2SO4	2.731-11	8.258-10	2.786-10	6.2640-9	4.486-10	9.3730-9	7.396-10	1.4260-8	1.2970-9	2.2750-8
NO	9.4443-5	1.4817-5	9.4442-5	1.4817-5	9.4442-5	1.4816-5	9.4441-5	1.4816-5	9.4441-5	1.4816-5
NO2	1.0011-6	5.1936-7	2.2385-6	1.1613-6	2.6487-6	1.3741-6	3.1657-6	1.6423-6	3.8772-6	2.0114-6
NO3	1.255-13	2.774-14	6.274-13	1.387-13	8.784-13	1.942-13	1.255-12	2.774-13	1.882-12	4.162-13
N2	7.3699-1	7.3703-1	7.3699-1	7.3703-1	7.3699-1	7.3703-1	7.3699-1	7.3703-1	7.3699-1	7.3703-1
N2O	5.5982-9	1.0091-9	1.2518-8	2.2563-9	1.4811-8	2.6697-9	1.7703-8	3.1909-9	2.1681-8	3.9081-9
NAOH	2.449-10	5.172-13	1.113-10	2.259-13	9.424-11	1.885-13	7.898-11	1.547-13	6.456-11	1.223-13
NA2SO4	3.224-13	1.411-13	6.791-13	2.043-13	7.839-13	2.128-13	9.078-13	2.179-13	1.064-12	2.175-13
O	3.4940-9	1.966-11	1.5630-9	8.794-12	1.3210-9	7.432-12	1.1050-9	6.218-12	9.022-10	5.077-12
OH	1.5471-6	5.5772-8	1.0346-6	3.7297-8	9.5112-7	3.4288-8	8.6998-7	3.1363-8	7.8611-7	2.8340-8
O2	6.6260-2	6.6300-2	6.6259-2	6.6299-2	6.6259-2	6.6299-2	6.6258-2	6.6299-2	6.6257-2	6.6298-2
O3	1.882-12	9.957-14	4.208-12	2.226-13	4.979-12	2.634-13	5.951-12	3.149-13	7.288-12	3.856-13
SO2	3.6779-6	2.4645-6	3.3561-6	1.6721-6	3.2615-6	1.5103-6	3.1494-6	1.3454-6	3.0071-6	1.1688-6
SO3	3.0907-7	1.5217-6	6.3064-7	2.3086-6	7.2513-7	2.4673-6	8.3691-7	2.6271-6	9.7868-7	2.7951-6
M, MOL WT	28.868	28.868	28.868	28.868	28.868	28.868	28.868	28.868	28.868	28.868
PHASE FRACTION	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0
SOLUTION 2										
NAOH(L)	2.0290-7	2.2686-8	4.6102-7	4.9553-8	5.4655-7	5.7883-8	6.5434-7	6.7846-8	8.0233-7	8.0469-8
NA2SO4(I)	0.000000	1.2589-3	0.000000	9.1129-3	0.000000	1.3289-2	0.000000	1.9440-2	0.000000	2.9096-2
NA2SO4(L)	4.8530-6	0.000000	5.1119-5	0.000000	8.2611-5	0.000000	1.3666-4	0.000000	2.4027-4	0.000000
NA2V2O6(L)	2.1162-1	2.2005-1	2.1700-1	2.1045-1	2.1765-1	2.0535-1	2.1821-1	1.9784-1	2.1858-1	1.8604-1
NA2V2O6(L)	2.1162-1	2.2005-1	2.1700-1	2.1045-1	2.1765-1	2.0535-1	2.1821-1	1.9784-1	2.1858-1	1.8604-1
NA4V2O7(S)	7.5883-8	1.2852-8	8.0339-8	1.1730-8	8.0895-8	1.1155-8	8.1371-8	1.0333-8	8.1700-8	9.1146-9
V2O3(S)	2.4650-6	1.1610-8	4.8960-7	2.3270-9	3.4940-7	1.6640-9	2.4440-7	1.1670-9	1.6280-7	7.802-10
V2O5(L)	7.8837-1	7.7870-1	7.8295-1	7.8044-1	7.8227-1	7.8136-1	7.8166-1	7.8272-1	7.8118-1	7.8486-1
M, MOL WT	195.00	195.47	195.33	194.56	195.37	194.08	195.40	193.37	195.42	192.25
PHASE FRACTION	1.2300-8	1.2315-8	1.2300-8	1.2413-8	1.2301-8	1.2465-8	1.2302-8	1.2544-8	1.2303-8	1.2668-8

PURE SPECIES PHASE FRACTIONS (IF ANY)

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-11 FOR ALL ASSIGNED CONDITI

SOLUTION 1

C	CH	CH2	CH2O	CH2O2	CH3	CH2OH	CH3O	CH4	CH
CN	CN2	CNN	COS	CS	CS2	C2	C2H	C2H2	C2
C2H4	C2H4O2	C2H4O4	C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3	C2N	C2
C2O	C3	C3H6O	N-C3H7	I-C3H7	C3H8	1-C3H7OH	C3O2	C4	C4
N-C4H10	I-C4H10	C4N2	C5	C4H5	C4H5O	C4H6	C4H5OH	C7H8	C8
N-C8H18	I-C8H18	O-C12H9	C12H10	HCN	HCO	HNCO	H2N2	H2S	N
NCO	NH	NH2	NH3	N2H4	N2O4	N2O5	N3	NA	NA
NAH	NAO	NA2	NA2CN2	NA2O	NA2O2H2	S	SH	SN	SO
S2	S2O	S8	V	VN	VO	VO2			

SOLUTION 2

NAOH(A)	NA2O(C)	NA2O(A)	NA2O(L)	NA2SO3(S)	NA2SO3(L)	NA2SO4(IV)	NA2V2O6(S)	NA4V2O8(S)	NA
V2O3(L)	V2O5(S)								

PURE SPECIES

C(GR)	C7H8(L)	C8H18(L)	H2O(S)	H2O(L)	H2SO4(L)	VN(S)	N2H6SO4(S)	NA(S)	NA
NACN(S)	NACN(L)	NAO2(S)	NA2O3(1)	NA2O3(2)	NA2O3(L)	NA2O2(A)	NA2O2(B)	NA2S(1)	NA
NA2S(L)	S(S)	S(L)	V(S)	V(L)	NAVSO8(S)	NA2V12O31(S)	NA2V12O31(L)	VO(S)	VO
VO2(S)	VO2(S)	VO2(L)							

CASE NO. 9701 212 0.01%SULFUR, 1.0 NA, 1.0 V PPM TIME = 0.702 SEC

P, ATM	1.0000	1.0000	5.0000	5.0000	7.0000	7.0000	10.000	10.000	15.000	15.000
T, DEG K	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0
SOLUTION 1										
AR	8.8005-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3
CO	3.0990-9	9.536-12	1.3860-9	4.265-12	1.1710-9	3.604-12	9.799-10	3.015-12	8.000-10	2.462-12
CO2	9.0898-2	9.0898-2	9.0898-2	9.0898-2	9.0898-2	9.0898-2	9.0898-2	9.0898-2	9.0898-2	9.0898-2
H	5.874-12	4.834-15	1.757-12	1.446-15	1.365-12	1.123-15	1.045-12	8.596-16	7.707-13	6.342-16
HNO	1.515-12	1.651-14	2.265-12	2.469-14	2.464-12	2.686-14	2.694-12	2.936-14	2.981-12	3.250-14
HNO2	4.1197-9	1.6058-9	1.3775-8	5.3694-9	1.7729-8	6.9107-9	2.3166-8	9.0302-9	3.1400-8	1.2237-8
HNO3	1.205-11	1.509-11	9.011-11	1.129-10	1.372-10	1.718-10	2.143-10	2.683-10	3.558-10	4.454-10
HO2	1.1950-8	9.702-10	1.7870-8	1.4510-9	1.9440-8	1.5780-9	2.1250-8	1.7250-9	2.3520-8	1.9090-9
H2	2.6140-9	1.618-11	1.1690-9	7.235-12	9.882-10	6.114-12	8.268-10	5.116-12	6.750-10	4.177-12
H2O	9.6947-2	9.6948-2	9.6947-2	9.6948-2	9.6947-2	9.6948-2	9.6947-2	9.6948-2	9.6947-2	9.6948-2
H2O2	4.817-10	5.487-11	1.0770-9	1.227-10	1.2750-9	1.452-10	1.5230-9	1.735-10	1.8660-9	2.125-10
H2SO4	2.729-11	8.227-10	2.779-10	6.2400-9	4.472-10	9.3350-9	7.372-10	1.4200-8	1.2930-9	2.2660-8
NO	9.4443-5	1.4817-5	9.4442-5	1.4817-5	9.4442-5	1.4816-5	9.4441-5	1.4816-5	9.4441-5	1.4816-5
NO2	1.0011-6	5.1936-7	2.2385-6	1.1613-6	2.6487-6	1.3741-6	3.1657-6	1.6423-6	3.8772-6	2.0114-6
NO3	1.255-13	2.774-14	6.274-13	1.387-13	8.784-13	1.942-13	1.255-12	2.774-13	1.882-12	4.162-13
N2	7.3699-1	7.3703-1	7.3699-1	7.3703-1	7.3699-1	7.3703-1	7.3699-1	7.3703-1	7.3699-1	7.3703-1
N2O	5.5982-9	1.0091-9	1.2518-8	2.2563-9	1.4811-8	2.6697-9	1.7703-8	3.1909-9	2.1681-8	3.9081-9
NA	2.980-12	3.457-17	3.465-13	1.695-18	1.956-13	9.138-19	1.035-13	4.773-19	4.910-14	2.296-19
NAOH	2.3040-8	1.082-11	8.9570-9	1.774-12	6.5080-9	1.231-12	4.5010-9	8.404-13	2.8930-9	5.479-13
NA2SO4	2.8500-9	6.157-11	4.3870-9	1.255-11	3.7280-9	9.043-12	2.9390-9	6.406-12	2.1290-9	4.346-12
O	3.4940-9	1.966-11	1.5630-9	8.794-12	1.3210-9	7.432-12	1.1050-9	6.218-12	9.022-10	5.077-12
OH	1.5471-6	5.5773-8	1.0346-6	3.7297-8	9.5112-7	3.4288-8	8.6998-7	3.1363-8	7.8611-7	2.8340-8
O2	6.6260-2	6.6300-2	6.6259-2	6.6299-2	6.6259-2	6.6299-2	6.6258-2	6.6299-2	6.6257-2	6.6298-2
O3	1.882-12	9.957-14	4.208-12	2.226-13	4.979-12	2.634-13	5.951-12	3.148-13	7.298-12	3.856-13
SO2	3.6748-6	2.4552-6	3.3473-6	1.6655-6	3.2519-6	1.5043-6	3.1394-6	1.3400-6	2.9969-6	1.1639-6
SO3	3.0881-7	1.5160-6	6.2898-7	2.2996-6	7.2300-7	2.4575-6	8.3425-7	2.6165-6	9.7536-7	2.7834-6
M, MOL WT	28.868	28.868	28.868	28.868	28.868	28.868	28.868	28.868	28.868	28.868
PHASE FRACTION	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0
SOLUTION 2										
NAOH(L)	1.9086-5	4.7472-7	3.7105-5	3.8912-7	3.7746-5	3.7806-7	3.7293-5	3.6860-7	3.5952-5	3.6048-7
NA2SO3(S)	0.000 0	5.011-12	0.000 0	2.284-12	0.000 0	1.947-12	0.000 0	1.649-12	0.000 0	1.370-12
NA2SO3(L)	1.553-10	0.000 0	5.345-10	0.000 0	5.374-10	0.000 0	5.064-10	0.000 0	4.493-10	0.000 0
NA2SO4(I)	0.000000	5.4922-1	0.000000	5.5976-1	0.000000	5.6464-1	0.000000	5.7146-1	0.000000	5.8145-1
NA2SO4(L)	4.2901-2	0.000000	3.3026-1	0.000000	3.9286-1	0.000000	4.4249-1	0.000000	4.8080-1	0.000000
NA2V2O6(L)	9.5365-1	4.4715-1	6.6773-1	4.1527-1	6.0557-1	3.9971-1	5.5618-1	3.7788-1	5.1785-1	3.4585-1
NA4V2O7(S)	3.0255-3	1.1437-5	1.6014-3	1.4272-6	1.0735-3	9.2623-7	6.7370-4	5.8267-7	3.8865-4	3.4003-7
NA6V2O8(S)	4.6751-8	0.000000	1.8705-8	0.000000	9.2689-9	0.000000	3.9746-9	0.000000	1.4206-9	0.000000
V2O3(S)	1.2550-9	5.388-11	2.326-10	7.447-11	2.038-10	7.594-11	1.918-10	7.553-11	1.921-10	7.227-11
V2O5(L)	4.0154-4	3.6136-3	3.7194-4	2.4974-2	4.5633-4	3.5652-2	6.1337-4	5.0653-2	9.2173-4	7.2705-2
M, MOL WT	239.65	187.71	210.30	185.32	203.89	184.16	198.80	182.53	194.86	180.15
PHASE FRACTION	1.2851-8	2.7286-8	1.8366-8	2.7939-8	2.0260-8	2.8252-8	2.2064-8	2.8702-8	2.3692-8	2.9387-8

PURE SPECIES PHASE FRACTIONS (IF ANY)

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-11 FOR ALL ASSIGNED CONDITI

SOLUTION 1

C	CH	CH2	CH2O	CH2O2	CH3	CH2OH	CH3O	CH4	CH
CN	CN2	CNN	COS	CS	CS2	C2	C2H	C2H2	C2
C2H4	C2H4O2	C2H4O4	C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3	C2N	C2
C2O	C3	C3H6O	N-C3H7	I-C3H7	C3H8	1-C3H7OH	C3O2	C4	C4
N-C4H10	I-C4H10	C4N2	C5	C6H5	C6H5O	C6H6	C6H5OH	C7H8	C8
N-C8H18	I-C8H18	O-C12H9	C12H10	HCN	HCO	HNCO	H2N2	H2S	N
NCO	NH	NH2	NH3	N2H4	N2O4	N2O5	NS	NAOH	NA
NAO	NA2	NA2(CN)2	NA2O	NA2(OH)2	S	SH	SN	SO	SO2
SO3	SO	V	VN	VO	VO2				

SOLUTION 2

NAOH(A)	NA2O(C)	NA2O(A)	NA2O(L)	NA2SO4(IV)	NA2V2O6(S)	NA6V2O8(L)	V2O3(L)	V2O5(S)	
PURE SPECIES									
C(GR)	C7H8(L)	C8H18(L)	H2O(S)	H2O(L)	H2SO4(L)	VN(S)	N2H6SO4(S)	NA(S)	NA
NAOH(S)	NAOH(L)	NAO2(S)	NA2O2(1)	NA2O2(2)	NA2O2(L)	NA2O2(A)	NA2O2(B)	NA2S(1)	NA
NA2S(L)	S(S)	S(L)	V(S)	V(L)	NAV3O8(S)	NA2V12O31(S)	NA2V12O31(L)	VO(S)	VO
VO2(S)	VO2(S)	VO2(L)							

CASE NO. B701 312 0.01%SULFUR, 10 NA, 1.0 V PPM TIME = 0.673 SEC

P, ATM	1.0000	1.0000	5.0000	5.0000	7.0000	7.0000	10.000	10.000	15.000	15.000
T, DEG K	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0
SOLUTION 1										
AR	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3
CO	3.0980-9	9.536-12	1.3860-9	4.265-12	1.1710-9	3.604-12	9.797-10	3.015-12	8.000-10	2.462-12
CO2	9.0897-2	9.0897-2	9.0897-2	9.0897-2	9.0897-2	9.0897-2	9.0897-2	9.0897-2	9.0897-2	9.0897-2
H	5.874-12	4.834-15	1.757-12	1.446-15	1.365-12	1.123-15	1.045-12	8.596-16	7.707-13	6.342-16
HNO	1.515-12	1.651-14	2.265-12	2.469-14	2.464-12	2.686-14	2.694-12	2.936-14	2.981-12	3.250-14
HNO2	4.1198-9	1.6059-9	1.3775-8	5.3695-9	1.7729-8	6.9108-9	2.3167-8	9.0303-9	3.1400-8	1.2240-8
HNO3	1.205-11	1.509-11	9.011-11	1.128-10	1.372-10	1.718-10	2.143-10	2.683-10	3.558-10	4.454-10
HO2	1.1950-8	9.702-10	1.7870-8	1.4510-9	1.9440-8	1.5780-9	2.1250-8	1.7250-9	2.3520-8	1.9090-9
H2	2.6140-9	1.618-11	1.1690-9	7.234-12	9.881-10	6.114-12	8.267-10	5.116-12	6.750-10	4.177-12
H2O	9.6946-2	9.6947-2	9.6947-2	9.6947-2	9.6947-2	9.6947-2	9.6947-2	9.6947-2	9.6947-2	9.6947-2
H2O2	4.817-10	5.487-11	1.0770-9	1.227-10	1.2750-9	1.452-10	1.5230-9	1.735-10	1.8660-9	2.125-10
H2SO4	2.591-11	7.719-10	2.610-10	5.8550-9	4.199-10	8.7600-9	6.919-10	1.3320-8	1.2130-9	2.1260-8
NO	9.4444-5	1.4817-5	9.4443-5	1.4817-5	9.4442-5	1.4817-5	9.4442-5	1.4817-5	9.4442-5	1.4817-5
NO2	1.0011-6	5.1937-7	2.2386-6	1.1613-6	2.6487-6	1.3741-6	3.1658-6	1.6423-6	3.8772-6	2.0114-6
NO3	1.255-13	2.775-14	6.274-13	1.387-13	8.784-13	1.942-13	1.255-12	2.774-13	1.882-12	4.162-13
N2	7.3699-1	7.3703-1	7.3699-1	7.3704-1	7.3699-1	7.3704-1	7.3699-1	7.3704-1	7.3699-1	7.3704-1
N2O	5.5983-9	1.0091-9	1.2518-8	2.2564-9	1.4811-8	2.6698-9	1.7703-8	3.1910-9	2.1682-8	3.9081-9
NA	1.417-11	4.705-17	6.068-13	2.285-18	3.144-13	1.227-18	1.569-13	6.369-19	7.138-14	3.037-19
NAO	1.684-12	9.143-18	1.613-13	9.929-19	9.886-14	6.307-19	5.896-14	3.914-19	3.286-14	2.286-19
NAOH	1.0950-7	1.473-11	1.5680-8	2.392-12	1.0460-8	1.653-12	6.8190-9	1.121-12	4.2060-9	7.249-13
NA2SO4	6.1170-8	1.070-10	1.2640-8	2.141-11	9.0370-9	1.529-11	6.3310-9	1.071-11	4.2230-9	7.138-12
O	3.4940-9	1.966-11	1.5630-9	8.794-12	1.3210-9	7.432-12	1.1050-9	6.218-12	9.022-10	5.077-12
OH	1.5471-6	5.5773-8	1.0346-6	3.7297-8	9.5112-7	3.4288-8	8.6998-7	3.1363-8	7.8611-7	2.8340-8
O2	6.6261-2	6.6302-2	6.6260-2	6.6301-2	6.6260-2	6.6300-2	6.6259-2	6.6300-2	6.6258-2	6.6300-2
O3	1.882-12	9.957-14	4.208-12	2.226-13	4.979-12	2.634-13	5.951-12	3.149-13	7.288-12	3.856-13
SO2	3.4891-6	2.3036-6	3.1437-6	1.5628-6	3.0529-6	1.4115-6	2.9465-6	1.2574-6	2.8124-6	1.0922-6
SO3	2.9321-7	1.4224-6	5.9073-7	2.1577-6	6.7876-7	2.3059-6	7.8301-7	2.4552-6	9.1531-7	2.6120-6
M, MOL WT	28.868	28.868	28.868	28.868	28.868	28.868	28.868	28.868	28.868	28.868
PHASE FRACTION	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0
SOLUTION 2										
NAOH(L)	9.0749-5	6.4621-7	6.4974-5	5.2469-7	6.0652-5	5.0756-7	5.6495-5	4.9190-7	5.2269-5	4.7693-7
NA2O(C)	1.693-11	0.000 0	1.736-12	0.000 0	1.081-12	0.000 0	0.000 0	0.000 0	0.000 0	0.000 0
NA2SO3(S)	0.000 0	8.712-12	0.000 0	3.896-12	0.000 0	3.293-12	0.000 0	2.755-12	0.000 0	2.250-12
NA2SO3(L)	3.3330-9	0.000 0	1.5390-9	0.000 0	1.3030-9	0.000 0	1.0910-9	0.000 0	8.913-10	0.000 0
NA2SO4(I)	0.000000	9.5486-1	0.000000	9.5493-1	0.000000	9.5496-1	0.000000	9.5501-1	0.000000	9.5509-1
NA2SO4(L)	9.2095-1	0.000000	9.5112-1	0.000000	9.5231-1	0.000000	9.5314-1	0.000000	9.5375-1	0.000000
NA2V2O6(L)	7.3670-2	4.4942-2	4.8446-2	4.3625-2	4.7400-2	4.2913-2	4.6654-2	4.1840-2	4.6091-2	4.0098-2
NA4V2O7(S)	5.2843-3	2.1299-6	3.5627-4	2.7260-7	2.1696-4	1.7923-7	1.2969-4	1.1490-7	7.3118-5	6.9007-8
NA6V2O8(S)	1.8460-6	0.000 0	1.2760-8	0.000 0	4.8370-9	0.000 0	1.7560-9	0.000 0	5.650-10	0.000 0
V2O3(S)	4.290-12	2.922-12	5.503-12	4.303-12	6.179-12	4.523-12	7.010-12	4.696-12	8.090-12	4.787-12
V2O5(L)	1.3720-6	1.9600-4	8.8003-6	1.4430-3	1.3833-5	2.1236-3	2.2419-5	3.1492-3	3.8811-5	4.8157-3
M, MOL WT	150.40	146.62	147.02	146.54	146.89	146.49	146.80	146.42	146.74	146.31
PHASE FRACTION	1.5578-7	2.7248-7	2.5198-7	2.7291-7	2.5823-7	2.7311-7	2.6278-7	2.7339-7	2.6621-7	2.7385-7

PURE SPECIES PHASE FRACTIONS (IF ANY)

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-11 FOR ALL ASSIGNED CONDITI

SOLUTION 1

C	CH	CH2	CH2O	CH2O2	CH3	CH2OH	CH3O	CH4	CH
CN	CN2	CNN	COS	CS	CS2	C2	C2H	C2H2	C2
C2H4	C2H4O2	C2H4O4	C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3	C2N	C2
C2O	C3	C3H6O	N-C3H7	I-C3H7	C3H8	1-C3H7OH	C3O2	C4	C4
N-C4H10	I-C4H10	C4N2	C5	C6H5	C6H5O	C6H6	C6H5OH	C7H8	C8
N-C8H18	I-C8H18	O-C12H9	C12H10	HCN	HCO	HNCO	H2N2	H2S	N
NCO	NH	NH2	NH3	N2H4	N2O4	N2O5	NS	NACN	NA
NA2	NA2C2N2	NA2O	NA2O2H2	S	SH	SN	SO	S2	S2

SB	V	VN	VO	VO2					
SOLUTION 2									
NAOH(A)	NA2O(A)	NA2O(L)	NA2SO4(IV)	NA2V2O6(S)	NA6V2O8(L)	V2O3(L)	V2O5(S)		
PURE SPECIES									
C(GR)	C7H8(L)	C8H18(L)	H2O(S)	H2O(L)	H2SO4(L)	VN(S)	N2H8SO4(S)	NA(S)	NA
NACN(S)	NACN(L)	NAO2(S)	NA2CO3(1)	NA2CO3(2)	NA2CO3(L)	NA2O2(A)	NA2O2(B)	NA2S(1)	NA
NA2S(L)	S(S)	S(L)	V(S)	V(L)	NAV3O8(S)	NA2V12O31(S)	NA2V12O31(L)	VO(S)	VO
VO2(S)	VO2(S)	VO2(L)							

CASE NO. 8701 113 0.01%SULFUR, 0.1 NA, 10. V PPM TIME = 0.483 SEC

P, ATM	1.0000	1.0000	5.0000	5.0000	7.0000	7.0000	10.000	10.000	15.000	15.000
T, DEG K	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0
SOLUTION 1										
AR	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3
CO	3.0980-9	9.536-12	1.3860-9	4.265-12	1.1710-9	3.604-12	9.797-10	3.015-12	8.000-10	2.462-12
CO2	9.0897-2	9.0897-2	9.0897-2	9.0897-2	9.0897-2	9.0897-2	9.0897-2	9.0897-2	9.0897-2	9.0897-2
H	5.874-12	4.834-15	1.757-12	1.446-15	1.365-12	1.123-15	1.045-12	8.596-16	7.707-13	6.342-16
HNO	1.515-12	1.651-14	2.265-12	2.469-14	2.464-12	2.686-14	2.694-12	2.936-14	2.981-12	3.250-14
HNO2	4.1198-9	1.6059-9	1.3775-8	5.3694-9	1.7729-8	6.9107-9	2.3167-8	9.0302-9	3.1400-8	1.2240-8
HNO3	1.205-11	1.509-11	9.011-11	1.128-10	1.372-10	1.718-10	2.143-10	2.683-10	3.558-10	4.454-10
HO2	1.1950-8	9.702-10	1.7870-8	1.4510-9	1.9440-8	1.5780-9	2.1250-8	1.7250-9	2.3520-8	1.9090-9
H2	2.6140-9	1.618-11	1.1690-9	7.235-12	9.881-10	6.114-12	8.267-10	5.116-12	6.750-10	4.177-12
H2O	9.6946-2	9.6947-2	9.6947-2	9.6947-2	9.6947-2	9.6947-2	9.6947-2	9.6947-2	9.6947-2	9.6947-2
H2O2	4.817-10	5.487-11	1.0770-9	1.227-10	1.2750-9	1.452-10	1.5230-9	1.735-10	1.8660-9	2.125-10
H2SO4	2.731-11	8.258-10	2.786-10	6.2640-9	4.486-10	9.3730-9	7.396-10	1.4260-8	1.2970-9	2.2750-8
NO	9.4444-5	1.4817-5	9.4443-5	1.4817-5	9.4442-5	1.4817-5	9.4442-5	1.4817-5	9.4441-5	1.4816-5
NO2	1.0011-6	5.1936-7	2.2386-6	1.1613-6	2.6487-6	1.3741-6	3.1658-6	1.6423-6	3.8772-6	2.0114-6
NO3	1.255-13	2.775-14	6.274-13	1.387-13	8.784-13	1.942-13	1.255-12	2.774-13	1.882-12	4.162-13
N2	7.3699-1	7.3703-1	7.3699-1	7.3703-1	7.3699-1	7.3703-1	7.3699-1	7.3703-1	7.3699-1	7.3703-1
N2O	5.5983-9	1.0091-9	1.2518-8	2.2564-9	1.4811-8	2.6698-9	1.7703-8	3.1910-9	2.1682-8	3.9081-9
NAOH	7.068-11	1.461-13	3.172-11	6.437-14	2.682-11	5.395-14	2.245-11	4.456-14	1.833-11	3.560-14
O	3.4940-9	1.966-11	1.5630-9	8.794-12	1.3210-9	7.432-12	1.1050-9	6.218-12	9.022-10	5.077-12
OH	1.5471-6	5.5773-8	1.0346-6	3.7297-8	9.5112-7	3.4288-8	8.6998-7	3.1363-8	7.8611-7	2.8340-8
O2	6.6261-2	6.6301-2	6.6260-2	6.6300-2	6.6260-2	6.6300-2	6.6259-2	6.6300-2	6.6258-2	6.6299-2
O3	1.882-12	9.957-14	4.208-12	2.226-13	4.979-12	2.634-13	5.951-12	3.149-13	7.288-12	3.856-13
SO2	3.6779-6	2.4644-6	3.3561-6	1.6721-6	3.2614-6	1.5103-6	3.1494-6	1.3454-6	3.0071-6	1.1688-6
SO3	3.0907-7	1.5217-6	6.3063-7	2.3086-6	7.2513-7	2.4673-6	8.3691-7	2.6271-6	9.7867-7	2.7952-6
M, MOL WT	28.868	28.868	28.868	28.868	28.868	28.868	28.868	28.868	28.868	28.868
PHASE FRACTION	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0
SOLUTION 2										
NAOH(L)	5.8561-8	6.4091-9	1.3142-7	1.4117-8	1.5556-7	1.6564-8	1.8599-7	1.9544-8	2.2783-7	2.3422-8
NA2SO4(I)	0.000000	1.0049-4	0.000000	7.3965-4	0.000000	1.0882-3	0.000000	1.6131-3	0.000000	2.4651-3
NA2SO4(L)	4.0424-7	0.000000	4.1539-6	0.000000	6.6922-6	0.000000	1.1041-5	0.000000	1.9374-5	0.000000
NA2V2O6(L)	2.1871-2	2.2056-2	2.2025-2	2.1402-2	2.2042-2	2.1046-2	2.2056-2	2.0509-2	2.2064-2	1.9639-2
NA4V2O7(S)	6.533-10	1.028-10	6.626-10	9.682-11	6.637-10	9.362-11	6.645-10	8.891-11	6.650-10	8.152-11
V2O3(S)	3.0580-6	1.4580-8	6.1150-7	2.9160-9	4.3680-7	2.0830-9	3.0580-7	1.4580-9	2.0380-7	9.721-10
V2O5(L)	9.7813-1	9.7784-1	9.7797-1	9.7786-1	9.7795-1	9.7787-1	9.7793-1	9.7788-1	9.7792-1	9.7790-1
M, MOL WT	183.24	183.24	183.24	183.18	183.25	183.14	183.25	183.09	183.25	183.00
PHASE FRACTION	1.2300-7	1.2301-7	1.2300-7	1.2309-7	1.2300-7	1.2313-7	1.2300-7	1.2320-7	1.2300-7	1.2330-7

PURE SPECIES PHASE FRACTIONS (IF ANY)

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-11 FOR ALL ASSIGNED CONDITI

SOLUTION 1

C	CH	CH2	CH2O	CH2O2	CH3	CH2OH	CH3O	CH4	CH
CN	CN2	CNN	COS	CS	CS2	C2	C2H	C2H2	C2
C2H4	C2H4O2	C2H4O4	C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3	C2N	C2
C2O	C3	C3H6O	N-C3H7	I-C3H7	C3H8	1-C3H7OH	C3O2	C4	C4
N-C4H10	I-C4H10	C4N2	C5	C6H5	C6H5O	C6H6	C6H5OH	C7H8	C8
N-C8H18	I-C8H18	O-C12H9	C12H10	HCN	HCO	HNCO	H2N2	H2S	N
NCO	NH	NH2	NH3	N2H4	N2O4	N2O5	N3	NA	NA
NAH	NAO	NA2	NA2C2N2	NA2O	NA2O2H2	NA2SO4	S	SH	SN
SO	S2	S2O	S8	V	VN	VO	VO2		

SOLUTION 2

NAOH(A)	NA2O(C)	NA2O(A)	NA2O(L)	NA2SO3(S)	NA2SO3(L)	NA2SO4(IV)	NA2V2O6(S)	NA6V2O8(S)	NA
V2O3(L)	V2O5(S)							

PURE SPECIES

C(GR)	C7H8(L)	C8H18(L)	H2O(S)	H2O(L)	H2SO4(L)	VN(S)	N2H6SO4(S)	NA(S)	NA
NACN(S)	NACN(L)	NAO2(S)	NA2CO3(1)	NA2CO3(2)	NA2CO3(L)	NA2O2(A)	NA2O2(B)	NA2S(1)	NA

NA2S(L)	S(S)	S(L)	V(S)	V(L)	NAV3O8(S)	NA2V12O31(S)	NA2V12O31(L)	VO(S)	VO
VO2(S)	VO2(S)	VO2(L)							

CASE NO. 8701 213 0.01%SULFUR, 1.0 NA, 10 V PPM TIME = 0.508 SEC

P, ATM	1.0000	1.0000	5.0000	5.0000	7.0000	7.0000	10.000	10.000	15.000	15.000
T, DEG K	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0
SOLUTION 1										
AR	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3
CO	3.0980-9	9.536-12	1.3860-9	4.265-12	1.1710-9	3.604-12	9.797-10	3.015-12	8.000-10	2.462-12
CO2	9.0897-2	9.0897-2	9.0897-2	9.0897-2	9.0897-2	9.0897-2	9.0897-2	9.0897-2	9.0897-2	9.0897-2
H	5.874-12	4.834-15	1.757-12	1.446-15	1.365-12	1.123-15	1.045-12	8.596-16	7.707-13	6.342-16
HNO	1.515-12	1.651-14	2.265-12	2.469-14	2.464-12	2.686-14	2.694-12	2.936-14	2.981-12	3.250-14
HNO2	4.1198-9	1.6059-9	1.3775-8	5.3695-9	1.7729-8	6.9107-9	2.3167-8	9.0302-9	3.1400-8	1.2240-8
HNO3	1.205-11	1.509-11	9.011-11	1.128-10	1.372-10	1.718-10	2.143-10	2.683-10	3.558-10	4.454-10
HO2	1.1950-8	9.702-10	1.7870-8	1.4510-9	1.9440-8	1.5780-9	2.1250-8	1.7250-9	2.3520-8	1.9090-9
H2	2.6140-9	1.618-11	1.1690-9	7.234-12	9.881-10	6.114-12	8.267-10	5.116-12	6.750-10	4.177-12
H2O	9.6946-2	9.6947-2	9.6946-2	9.6947-2	9.6947-2	9.6947-2	9.6947-2	9.6947-2	9.6947-2	9.6947-2
H2O2	4.817-10	5.487-11	1.0770-9	1.227-10	1.2750-9	1.452-10	1.5230-9	1.735-10	1.8660-9	2.125-10
H2SO4	2.731-11	8.258-10	2.786-10	6.2630-9	4.486-10	9.3690-9	7.396-10	1.4250-8	1.2970-9	2.2730-8
NO	9.4444-5	1.4817-5	9.4443-5	1.4817-5	9.4442-5	1.4817-5	9.4442-5	1.4817-5	9.4441-5	1.4817-5
NO2	1.0011-6	5.1937-7	2.2386-6	1.1613-6	2.6487-6	1.3741-6	3.1658-6	1.6423-6	3.8772-6	2.0114-6
NO3	1.255-13	2.775-14	6.274-13	1.387-13	8.784-13	1.942-13	1.255-12	2.774-13	1.882-12	4.162-13
N2	7.3699-1	7.3703-1	7.3699-1	7.3703-1	7.3699-1	7.3703-1	7.3699-1	7.3703-1	7.3699-1	7.3703-1
N2O	5.5983-9	1.0091-9	1.2518-8	2.2564-9	1.4811-8	2.6698-9	1.7703-8	3.1910-9	2.1682-8	3.9081-9
NAOH	2.514-10	5.172-13	1.126-10	2.259-13	9.519-11	1.885-13	7.965-11	1.547-13	6.502-11	1.223-13
NA2SO4	3.398-13	1.411-13	6.954-13	2.043-13	7.998-13	2.127-13	9.232-13	2.178-13	1.079-12	2.173-13
O	3.4940-9	1.966-11	1.5630-9	8.794-12	1.3210-9	7.432-12	1.1050-9	6.218-12	9.022-10	5.077-12
OH	1.5471-6	5.5773-8	1.0346-6	3.7297-8	9.5112-7	3.4288-8	8.6998-7	3.1363-8	7.8611-7	2.8340-8
O2	6.6261-2	6.6301-2	6.6260-2	6.6300-2	6.6260-2	6.6300-2	6.6259-2	6.6300-2	6.6258-2	6.6299-2
O3	1.882-12	9.957-14	4.208-12	2.226-13	4.979-12	2.634-13	5.951-12	3.149-13	7.288-12	3.856-13
SO2	3.6779-6	2.4644-6	3.3561-6	1.6716-6	3.2614-6	1.5097-6	3.1494-6	1.3447-6	3.0070-6	1.1678-6
SO3	3.0907-7	1.5217-6	6.3063-7	2.3080-6	7.2513-7	2.4663-6	8.3691-7	2.6256-6	9.7867-7	2.7928-6
M, MOL WT	28.868	28.868	28.868	28.868	28.868	28.868	28.868	28.868	28.868	28.868
PHASE FRACTION	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0
SOLUTION 2										
NAOH(L)	2.0832-7	2.2685-8	4.6653-7	4.9553-8	5.5207-7	5.7883-8	6.5986-7	6.7848-8	8.0804-7	8.0474-8
NA2SO4(I)	0.000000	1.2589-3	0.000000	9.1107-3	0.000000	1.3284-2	0.000000	1.9430-2	0.000000	2.9075-2
NA2SO4(L)	5.1158-6	0.000000	5.2348-5	0.000000	8.4288-5	0.000000	1.3898-4	0.000000	2.4370-4	0.000000
NA2SO4(L)	5.1158-6	0.000000	5.2348-5	0.000000	8.4288-5	0.000000	1.3898-4	0.000000	2.4370-4	0.000000
NA2V2O6(L)	2.2053-1	2.2005-1	2.2106-1	2.1045-1	2.2109-1	2.0536-1	2.2109-1	1.9785-1	2.2101-1	1.8607-1
NA4V2O7(S)	8.3369-8	1.2852-8	8.3812-8	1.1730-8	8.3843-8	1.1135-8	8.3846-8	1.0336-8	8.3790-8	9.1171-9
V2O3(S)	2.4370-6	1.1610-8	4.8710-7	2.3270-9	3.4790-7	1.6640-9	2.4350-7	1.1670-9	1.6230-7	7.802-10
V2O5(L)	7.7944-1	7.7870-1	7.7889-1	7.8044-1	7.7882-1	7.8136-1	7.7877-1	7.8272-1	7.7874-1	7.8486-1
M, MOL WT	195.55	195.47	195.58	194.56	195.58	194.08	195.58	193.37	195.57	192.25
PHASE FRACTION	1.2300-7	1.2315-7	1.2300-7	1.2413-7	1.2301-7	1.2465-7	1.2301-7	1.2543-7	1.2303-7	1.2668-7

PURE SPECIES PHASE FRACTIONS (IF ANY)

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-11 FOR ALL ASSIGNED CONDITI

SOLUTION 1

C	CH	CH2	CH2O	CH2O2	CH3	CH2OH	CH3O	CH4	CH
CN	CN2	CNN	COS	CS	CS2	C2	C2H	C2H2	C2
C2H4	C2H4O2	C2H4O4	C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3	C2N	C2
C2O	C3	C3H6O	N-C3H7	I-C3H7	C3H8	1-C3H7OH	C3O2	C4	C4
N-C4H10	I-C4H10	C4N2	C5	C6H5	C6H5O	C6H6	C6H5OH	C7H8	C8
N-C8H18	I-C8H18	O-C12H9	C12H10	HCN	HCO	HNCO	H2N2	H2S	N
NCO	NH	NH2	NH3	N2H4	N2O4	N2O5	N3	NA	NA
NAH	NAO	NA2	NA2C2N2	NA2O	NA2O2H2	S	SH	SN	SO
SO2	SO3	SS	V	VN	VO	VO2			

SOLUTION 2

NAOH(A)	NA2O(C)	NA2O(A)	NA2O(L)	NA2SO3(S)	NA2SO3(L)	NA2SO4(IV)	NA2V2O6(S)	NA6V2O8(S)	NA
V2O3(L)	V2O5(S)								

PURE SPECIES

C(GR)	C7H8(L)	C8H18(L)	H2O(S)	H2O(L)	H2SO4(L)	VN(S)	N2H6SO4(S)	NA(S)	NA
NACN(S)	NACN(L)	NAO2(S)	NA2CO3(I)	NA2CO3(2)	NA2CO3(L)	NA2O2(A)	NA2O2(B)	NA2S(I)	NA
NA2S(L)	S(S)	S(L)	V(S)	V(L)	NAV3O8(S)	NA2V12O31(S)	NA2V12O31(L)	VO(S)	VO
VO2(S)	VO2(S)	VO2(L)							

CASE NO. 8701 313 0.01%SULFUR, 10 NA, 10. V PPM TIME = 0.677 SEC

P, ATM	1.0000	1.0000	5.0000	5.0000	7.0000	7.0000	10.000	10.000	15.000	15.000
T, DEG K	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0
SOLUTION 1										
AR	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3	8.8006-3
CO	3.0980-9	9.536-12	1.3860-9	4.264-12	1.1710-9	3.604-12	9.797-10	3.015-12	7.999-10	2.462-12
CO2	9.0896-2	9.0896-2	9.0896-2	9.0896-2	9.0896-2	9.0897-2	9.0896-2	9.0897-2	9.0897-2	9.0897-2
H	5.874-12	4.834-15	1.757-12	1.446-15	1.365-12	1.123-15	1.045-12	8.596-16	7.707-13	6.342-16
HNO	1.515-12	1.651-14	2.265-12	2.469-14	2.464-12	2.686-14	2.694-12	2.936-14	2.981-12	3.250-14
HNO2	4.1198-9	1.6059-9	1.3775-8	5.3695-9	1.7729-8	6.9108-9	2.3167-8	9.0303-9	3.1400-8	1.2240-8
HNO3	1.205-11	1.509-11	9.011-11	1.128-10	1.372-10	1.718-10	2.143-10	2.683-10	3.358-10	4.454-10
HO2	1.1950-8	9.702-10	1.7870-8	1.4510-9	1.9440-8	1.5780-9	2.1250-8	1.7250-9	2.3520-8	1.9090-9
H2	2.6140-9	1.618-11	1.1690-9	7.234-12	9.881-10	6.114-12	8.267-10	5.116-12	6.750-10	4.177-12
H2O	9.6945-2	9.6946-2	9.6946-2	9.6946-2	9.6946-2	9.6946-2	9.6946-2	9.6946-2	9.6946-2	9.6946-2
H2O2	4.817-10	5.487-11	1.0770-9	1.227-10	1.2750-9	1.452-10	1.5230-9	1.735-10	1.8660-9	2.125-10
H2SO4	2.656-11	7.946-10	2.686-10	6.0190-9	4.322-10	8.9980-9	7.123-10	1.3670-8	1.2490-9	2.1780-8
NO	9.4444-5	1.4817-5	9.4443-5	1.4817-5	9.4443-5	1.4817-5	9.4443-5	1.4817-5	9.4442-5	1.4817-5
NO2	1.0012-6	5.1937-7	2.2386-6	1.1613-6	2.6487-6	1.3741-6	3.1658-6	1.6424-6	3.8773-6	2.0115-6
NO3	1.255-13	2.775-14	6.274-13	1.387-13	8.784-13	1.942-13	1.255-12	2.775-13	1.882-12	4.162-13
N2	7.3699-1	7.3704-1	7.3699-1	7.3704-1	7.3699-1	7.3704-1	7.3699-1	7.3704-1	7.3699-1	7.3704-1
N2O	5.5983-9	1.0091-9	1.2518-8	2.2564-9	1.4812-8	2.6698-9	1.7703-8	3.1910-9	2.1682-8	3.9081-9
NA	9.265-12	3.520-17	4.447-13	1.725-18	2.318-13	9.304-19	1.162-13	4.861-19	5.304-14	2.340-19
NAO	1.101-12	6.840-18	1.182-13	7.497-19	7.290-14	4.784-19	4.367-14	2.987-19	2.442-14	1.761-19
NAOH	7.1620-8	1.102-11	1.1490-8	1.806-12	7.7120-9	1.254-12	5.0500-9	8.559-13	3.1250-9	5.584-13
NA2SO4	2.6810-8	6.168-11	6.9840-9	1.255-11	5.0580-9	9.037-12	3.5750-9	6.400-12	2.4010-9	4.339-12
O	3.4940-9	1.966-11	1.5630-9	8.794-12	1.3210-9	7.432-12	1.1050-9	6.218-12	9.022-10	5.077-12
OH	1.5471-6	5.5773-8	1.0346-6	3.7297-8	9.5112-7	3.4288-8	8.6998-7	3.1363-8	7.8611-7	2.8340-8
O2	6.6262-2	6.6302-2	6.6261-2	6.6302-2	6.6261-2	6.6301-2	6.6260-2	6.6301-2	6.6259-2	6.6300-2
O3	1.882-12	9.957-14	4.208-12	2.226-13	4.979-12	2.634-13	5.951-12	3.149-13	7.288-12	3.856-13
SO2	3.5763-6	2.3714-6	3.2354-6	1.6065-6	3.1424-6	1.4499-6	3.0333-6	1.2903-6	2.8954-6	1.1190-6
SO3	3.0054-7	1.4643-6	6.0796-7	2.2182-6	6.9867-7	2.3688-6	8.0606-7	2.5194-6	9.4233-7	2.6760-6
M, MOL WT	28.868	28.868	28.868	28.868	28.868	28.868	28.868	28.868	28.868	28.868
PHASE FRACTION	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0
SOLUTION 2										
NAOH(L)	5.9341-5	4.8344-7	4.7617-5	3.9614-7	4.4723-5	3.8494-7	4.1841-5	3.7543-7	3.8839-5	3.6736-7
NA2O(C)	7.241-12	0.000 0	0.000 0	0.000 0	0.000 0	0.000 0	0.000 0	0.000 0	0.000 0	0.000 0
NA2SO3(S)	0.000 0	5.019-12	0.000 0	2.283-12	0.000 0	1.946-12	0.000 0	1.647-12	0.000 0	1.368-12
NA2SO3(L)	1.4610-9	0.000 0	8.509-10	0.000 0	7.291-10	0.000 0	6.160-10	0.000 0	5.066-10	0.000 0
NA2SO4(I)	0.000000	5.5016-1	0.000000	5.5958-1	0.000000	5.6426-1	0.000000	5.7085-1	0.000000	5.8056-1
NA2SO4(L)	4.0363-1	0.000000	5.2574-1	0.000000	5.3299-1	0.000000	5.3820-1	0.000000	5.4215-1	0.000000
NA2V2O6(L)	5.7854-1	4.4635-1	4.7218-1	4.1626-1	4.6556-1	4.0122-1	4.6065-1	3.8004-1	4.5672-1	3.4883-1
NA4V2O7(S)	1.7744-2	1.1839-5	1.8650-3	1.4827-6	1.1587-3	9.6391-7	7.0240-4	6.0792-7	4.0005-4	3.5619-7
NA6V2O8(S)	2.6506-6	0.000000	3.5878-8	0.000000	1.4045-8	0.000000	5.2165-9	0.000000	1.7067-9	0.000000
V2O3(S)	7.878-11	5.186-11	9.986-11	7.203-11	1.116-10	7.352-11	1.262-10	7.322-11	1.452-10	7.019-11
V2O5(L)	2.5198-5	3.4781-3	1.5970-4	2.4154-2	2.4989-4	3.4517-2	4.0357-4	4.9105-2	6.9653-4	7.0609-2
M, MOL WT	203.85	187.63	190.42	185.38	189.64	184.27	189.07	182.69	188.63	180.37
PHASE FRACTION	2.0626-7	2.7342-7	2.5937-7	2.7927-7	2.6339-7	2.8227-7	2.6636-7	2.8661-7	2.6866-7	2.9324-7

PURE SPECIES PHASE FRACTIONS (IF ANY)

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-11 FOR ALL ASSIGNED CONDITI

SOLUTION 1

C	CH	CH2	CH2O	CH2O2	CH3	CH2OH	CH3O	CH4	CH
CN	CN2	CNN	COS	CS	CS2	C2	C2H	C2H2	C2
C2H4	C2H4O2	C2H4O4	C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3	C2N	C2
C2O	C3	C3H6O	N-C3H7	I-C3H7	C3H8	1-C3H7OH	C3O2	C4	C4
N-C4H10	I-C4H10	C4N2	C5	C6H5	C6H5O	C6H6	C6H5OH	C7H8	C8
N-C8H18	I-C8H18	O-C12H9	C12H10	HCN	HCO	HNCO	H2N2	H2S	N
NCO	NH	NH2	NH3	N2H4	N2O4	N2O5	N3	NACN	NA
NA2	NA2C2N2	NA2O	NA2O2H2	S	SH	SN	SO	S2	S2

S8	V	VN	VO	VO2				
SOLUTION 2								
NAOH(A)	NA2O(A)	NA2O(L)	NA2SO4(IV)	NA2V2O6(S)	NA6V2O8(L)	V2O3(L)	V2O5(S)	
PURE SPECIES								
C(GR)	C7H8(L)	C8H18(L)	H2O(S)	H2O(L)	H2SO4(L)	VN(S)	NH4HSO4(S)	NA(S)	NA
NACN(S)	NACN(L)	NAO2(S)	NA2CO3(1)	NA2CO3(2)	NA2CO3(L)	NA2O2(A)	NA2O2(B)	NA2S(1)	NA
NA2S(L)	S(S)	S(L)	V(S)	V(L)	NAV3O8(S)	NA2V12O31(S)	NA2V12O31(L)	VO(S)	VO
VO2(S)	VO2(S)	VO2(L)							

STOP

V01S&NV V-NA SYSTEMS TO DEVELOP CORROSION TH 01/87

SOLN 1 GASES

SOLN 2 V2O5(L) V2O3(L) V2O4(L) VCL4(L)
SOLN 2 NA2SO3(L) NA2SO4(L) NAOH(L)
SOLN 2 NA2O(L) NA2V2O6(S) NA4V2O7(S) NA6V2O8(S)

CASE NO. 8701 121 0.1% SULFUR, 0.1 NA, 0.1 V PPM singular matrix, iteration 40 variable 7

P, ATM	1.0000	1.0000	7.0000	7.0000
T, DEG K	1172.0	977.0	1172.0	977.0
SOLUTION 1				
AR	8.8009-3	8.8009-3	8.8009-3	8.8010-3
CO	3.0930-9	9.522-12	1.1690-9	3.599-12
CO2	9.0818-2	9.0819-2	9.0819-2	9.0819-2
H	5.870-12	4.831-15	1.364-12	1.123-15
HNO	1.515-12	1.651-14	2.464-12	2.686-14
HNO2	4.1223-9	1.6068-9	1.7740-8	6.9143-9
HNO3	1.207-11	1.511-11	1.374-10	1.720-10
HO2	1.1960-8	9.707-10	1.9450-8	1.5790-9
H2	2.6110-9	1.616-11	9.868-10	6.106-12
H2O	9.6876-2	9.6877-2	9.6876-2	9.6878-2
H2O2	4.817-10	5.487-11	1.2740-9	1.452-10
H2SO4	2.729-10	8.2480-9	4.4810-9	9.3600-8
NO	9.4506-5	1.4826-5	9.4503-5	1.4825-5
NO2	1.0024-6	5.2000-7	2.6521-6	1.3757-6
N2	7.3702-1	7.3707-1	7.3702-1	7.3707-1
N2O	5.6021-9	1.0097-9	1.4821-8	2.6714-9
NAOH	2.4320-9	3.428-12	1.0090-9	4.083-13
NA2SO4	3.181-10	6.203-11	8.994-10	9.984-12
O	3.4960-9	1.968-11	1.3210-9	7.437-12
OH	1.5470-6	5.5769-8	9.5107-7	3.4286-8
O2	6.6346-2	6.6381-2	6.6343-2	6.6376-2
O3	1.885-12	9.975-14	4.988-12	2.639-13
SO2	3.6745-5	2.4617-5	3.2582-5	1.5084-5
SO3	3.0899-6	1.5209-5	7.2485-6	2.4656-5
M, MOL WT	28.869	28.869	28.869	28.869
PHASE FRACTION	1.0000 0	1.0000 0	1.0000 0	1.0000 0
SOLUTION 2				
NAOH(L)	2.0152-6	1.5037-7	5.8532-6	1.2537-7
NA2SO3(S)	0.000 0	5.045-12	0.000 0	2.149-12
NA2SO3(L)	1.732-11	0.000 0	1.296-10	0.000 0
NA2SO4(I)	0.000000	5.5327-1	0.000000	6.2341-1
NA2SO4(L)	4.7891-3	0.000000	9.4780-2	0.000000
NA2V2O6(L)	9.5898-1	4.1345-1	8.7769-1	2.0800-1
NA4V2O7(S)	3.3944-5	1.0618-6	3.7441-5	5.3040-8
NA6V2O8(S)	5.852-12	0.000 0	7.779-12	0.000 0
V2O3(S)	1.1300-7	4.955-10	1.2260-8	3.587-10
V2O5(L)	3.6192-2	3.3275-2	2.7485-2	1.6859-1
M, MOL WT	241.13	185.46	232.51	169.93
PHASE FRACTION	1.2360-9	2.7534-9	1.3588-9	3.2663-9

PURE SPECIES PHASE FRACTIONS (IF ANY)
ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-11 FOR ALL ASSIGNED CONDITI
SOLUTION 1

C	CH	CH2	CH2O	CH2O2	CH3	CH2OH	CH3O	CH4	CH
CN	CN2	CNN	COS	CS	CS2	C2	C2H	C2H2	C2
C2H4	C2H4O2	C2H4O4	C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3	C2N	C2
C2O	C3	C3H6O	N-C3H7	I-C3H7	C3H8	1-C3H7OH	C3O2	C4	C4

N-C4H10	I-C4H10	C4N2	CS	C6H5	C6H5O	C6H6	C6H5OH	C7H8	C8
N-C8H18	I-C8H18	O-C12H9	C12H10	HCN	HCO	HNCO	H2N2	H2S	N
NCO	NH	NH2	NH3	NO3	N2H4	N2O4	N2O5	NS	NA
NACN	NAH	NAO	NA2	NA2C2N2	NA2O	NA2O2H2	S	SH	SN
SO	S2	S2O	S8	V	VN	VO	VO2		

SOLUTION 2

NAOH(A)	NA2O(C)	NA2O(A)	NA2O(L)	NA2SO4(IV)	NA2V2O6(S)	NA6V2O8(L)	V2O3(L)	V2O5(S)

PURE SPECIES

C(GR)	C7H8(L)	C8H18(L)	H2O(S)	H2O(L)	H2SO4(L)	VN(S)	N2H8SO4(S)	NA(S)	NA
NACN(S)	NACN(L)	NAO2(S)	NA2CO3(1)	NA2CO3(2)	NA2CO3(L)	NA2O2(A)	NA2O2(B)	NA2S(1)	NA
NA2S(L)	S(S)	S(L)	V(S)	V(L)	NAV3O8(S)	NA2V12O31(S)	NA2V12O31(L)	VO(S)	VO
VO2(S)	VO2(S)	VO2(L)							

CASE NO. 8701 221 0.1% SULFUR, 1.0 NA, 0.1 V PPM TIME = 0.611 SEC

P, ATM	1.0000	1.0000	7.0000	7.0000	10.000	10.000	15.000	15.000
T, DEG K	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0
SOLUTION 1								
AR	8.8009-3	8.8009-3	8.8009-3	8.8010-3	8.8009-3	8.8010-3	8.8009-3	8.8010-3
CO	3.0930-9	9.522-12	1.1690-9	3.599-12	9.783-10	3.011-12	7.988-10	2.459-12
CO2	9.0818-2	9.0819-2	9.0819-2	9.0819-2	9.0819-2	9.0819-2	9.0819-2	9.0820-2
H	5.870-12	4.831-15	1.364-12	1.123-15	1.044-12	8.591-16	7.702-13	6.338-16
HNO	1.515-12	1.651-14	2.464-12	2.686-14	2.694-12	2.936-14	2.981-12	3.249-14
HNO2	4.1223-9	1.6068-9	1.7740-8	6.9143-9	2.3180-8	9.0349-9	3.1418-8	1.2246-8
HNO3	1.207-11	1.511-11	1.374-10	1.720-10	2.146-10	2.686-10	3.562-10	4.459-10
HO2	1.1960-8	9.707-10	1.9450-8	1.5790-9	2.1260-8	1.7260-9	2.3530-8	1.9100-9
H2	2.6110-9	1.616-11	9.868-10	6.106-12	8.256-10	5.109-12	6.741-10	4.172-12
H2O	9.6876-2	9.6877-2	9.6876-2	9.6878-2	9.6877-2	9.6878-2	9.6877-2	9.6878-2
H2O2	4.817-10	5.487-11	1.2740-9	1.452-10	1.5230-9	1.735-10	1.8650-9	2.125-10
H2SO4	2.727-10	8.2430-9	4.4780-9	9.3540-8	7.3830-9	1.4230-7	1.2950-8	2.2710-7
NO	9.4506-5	1.4826-5	9.4503-5	1.4825-5	9.4503-5	1.4825-5	9.4502-5	1.4825-5
NO2	1.0024-6	5.2000-7	2.6521-6	1.3757-6	3.1698-6	1.6442-6	3.8821-6	2.0137-6
NO3	1.257-13	2.780-14	8.801-13	1.946-13	1.257-12	2.779-13	1.886-12	4.169-13
N2	7.3702-1	7.3707-1	7.3702-1	7.3707-1	7.3702-1	7.3707-1	7.3702-1	7.3707-1
N2O	5.6021-9	1.0097-9	1.4821-8	2.6714-9	1.7715-8	3.1929-9	2.1696-8	3.9105-9
NA	2.285-12	1.439-17	9.491-14	3.753-19	4.762-14	1.949-19	2.174-14	9.293-20
NAOH	1.7670-8	4.505-12	3.1570-9	5.057-13	2.0700-9	3.431-13	1.2810-9	2.218-13
NA2SO4	1.6770-8	1.070-10	8.7980-9	1.530-11	6.2340-9	1.071-11	4.1850-9	7.145-12
O	3.4960-9	1.968-11	1.3210-9	7.437-12	1.1060-9	6.222-12	9.027-10	5.080-12
OH	1.5470-6	5.5769-8	9.5107-7	3.4286-8	8.6994-7	3.1361-8	7.8607-7	2.8337-8
O2	6.6346-2	6.6381-2	6.6343-2	6.6376-2	6.6342-2	6.6375-2	6.6340-2	6.6374-2
O3	1.885-12	9.975-14	4.988-12	2.639-13	5.962-12	3.154-13	7.302-12	3.863-13
SO2	3.6729-5	2.4601-5	3.2562-5	1.5075-5	3.1443-5	1.3430-5	3.0021-5	1.1667-5
SO3	3.0885-6	1.5200-5	7.2443-6	2.4641-5	8.3607-6	2.6238-5	9.7766-6	2.7916-5
M, MOL WT	28.869	28.869	28.869	28.869	28.869	28.869	28.869	28.869
PHASE FRACTION	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0
SOLUTION 2								
NAOH(L)	1.4636-5	1.9760-7	1.8312-5	1.5526-7	1.7149-5	1.5048-7	1.5916-5	1.4590-7
NA2SO3(S)	0.000 0	8.706-12	0.000 0	3.293-12	0.000 0	2.756-12	0.000 0	2.251-12
NA2SO3(L)	9.134-10	0.000 0	1.2670-9	0.000 0	1.0730-9	0.000 0	8.827-10	0.000 0
NA2SO4(I)	0.000000	9.5478-1	0.000000	9.5554-1	0.000000	9.5574-1	0.000000	9.5598-1
NA2SO4(L)	2.5253-1	0.000000	9.2712-1	0.000000	9.3846-1	0.000000	9.4517-1	0.000000
NA2V2O6(L)	7.4553-1	4.3206-2	7.2595-2	2.9088-2	6.1188-2	2.4537-2	5.4312-2	1.9289-2
NA4V2O7(S)	1.3921-3	1.9160-7	3.0311-5	1.1376-8	1.5685-5	6.3100-9	7.9940-6	3.1090-9
NA6V2O8(S)	1.2660-8	0.000 0	6.164-11	0.000 0	1.958-11	0.000 0	5.731-12	0.000 0
V2O3(S)	1.6650-9	2.999-11	1.036-10	3.271-11	9.958-11	2.937-11	1.026-10	2.456-11
V2O5(L)	5.3336-4	2.0138-3	2.3226-4	1.5373-2	3.1887-4	1.9721-2	4.9292-4	2.4736-2
M, MOL WT	218.20	146.52	149.44	145.61	148.28	145.32	147.59	144.99
PHASE FRACTION	1.6456-9	2.7201-8	1.6883-8	2.7666-8	1.9993-8	2.7793-8	2.2441-8	2.7940-8

PURE SPECIES PHASE FRACTIONS (IF ANY)

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-11 FOR ALL ASSIGNED CONDITI

SOLUTION 1

C	CH	CH2	CH2O	CH2O2	CH3	CH2OH	CH3O	CH4	CH
CN	CN2	CNN	COS	CS	CS2	C2	C2H	C2H2	C2
C2H4	C2H4O2	C2H4O4	C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3	C2N	C2
C2O	C3	C3H6O	N-C3H7	I-C3H7	C3H8	1-C3H7OH	C3O2	C4	C4
N-C4H10	I-C4H10	C4N2	C5	C6H5	C6H5O	C6H6	C6H5OH	C7H8	C8
N-C8H18	I-C8H18	O-C12H9	C12H10	HCN	HCO	HNCO	H2N2	H2S	N
NCO	NH	NH2	NH3	N2H4	N2O4	N2O5	N3	NACN	NA
NAO	NA2	NA2C2N2	NA2O	NA2O2H2	S	SH	SN	SO	S2
S2O	S8	V	VN	VO	VO2				

SOLUTION 2

NAOH(A)	NA2O(C)	NA2O(A)	NA2O(L)	NA2SO4(IV)	NA2V2O6(S)	NA6V2O8(L)	V2O3(L)	V2O5(S)
PURE SPECIES								
C(GR)	C7H8(L)	C8H18(L)	H2O(S)	H2O(L)	H2SO4(L)	VN(S)	N2H6SO4(S)	NA(S)
NACN(S)	NACN(L)	NAO2(S)	NA2CO3(I)	NA2CO3(2)	NA2CO3(L)	NA2O2(A)	NA2O2(B)	NA2S(I)
NA2S(L)	S(S)	S(L)	V(S)	V(L)	NAV3O8(S)	NA2V12O31(S)	NA2V12O31(L)	VO(S)	VO
VO2(S)	VO2(S)	VO2(L)						

CASE NO. 8701 321 0.1% SULFUR, 10 NA, 0.1 V PPM 182 iterations did not satisfy convergence requirements

P, ATM	1.0000	1.0000	7.0000	7.0000
T, DEG K	1172.0	977.0	1172.0	977.0
SOLUTION 1				
AR	8.8009-3	8.8010-3	8.8009-3	8.8010-3
CO	3.0930-9	9.522-12	1.1690-9	3.599-12
CO2	9.0818-2	9.0818-2	9.0818-2	9.0819-2
H	5.870-12	4.831-15	1.364-12	1.123-15
HNO	1.515-12	1.651-14	2.464-12	2.686-14
HNO2	4.1223-9	1.6068-9	1.7740-8	6.9144-9
HNO3	1.207-11	1.511-11	1.374-10	1.720-10
HO2	1.1960-8	9.707-10	1.9450-8	1.5790-9
H2	2.6110-9	1.616-11	9.868-10	6.106-12
H2O	9.6875-2	9.6877-2	9.6876-2	9.6877-2
H2O2	4.817-10	5.487-11	1.2740-9	1.452-10
H2SO4	2.711-10	8.1920-9	4.4500-9	9.2960-8
NO	9.4507-5	1.4826-5	9.4504-5	1.4826-5
NO2	1.0025-6	5.2001-7	2.6521-6	1.3757-6
N2	7.3702-1	7.3707-1	7.3702-1	7.3707-1
N2O	5.6021-9	1.0097-9	1.4821-8	2.6714-9
NA	4.546-12	1.474-17	9.864-14	3.843-19
NAOH	3.5140-8	4.614-12	3.2820-9	5.177-13
NA2SO4	6.5990-8	1.116-10	9.4440-9	1.594-11
O	3.4960-9	1.968-11	1.3210-9	7.437-12
OH	1.5470-6	5.5769-8	9.5107-7	3.4286-8
O2	6.6347-2	6.6382-2	6.6344-2	6.6377-2
O3	1.886-12	9.975-14	4.988-12	2.639-13
SO2	3.6511-5	2.4450-5	3.2361-5	1.4982-5
SO3	3.0702-6	1.5106-5	7.1996-6	2.4489-5
M, MOL WT	28.869	28.869	28.869	28.869
PHASE FRACTION	1.0000 0	1.0000 0	1.0000 0	1.0000 0
SOLUTION 2				
NAOH(L)	2.9117-5	2.0239-7	1.9032-5	1.5896-7
NA2O(C)	1.745-12	0.000 0	0.000 0	0.000 0
NA2SO3(S)	0.000 0	9.077-12	0.000 0	3.431-12
NA2SO3(L)	3.5932-9	0.000000	1.3606-9	0.000000
NA2SO4(I)	0.000000	9.9549-1	0.000000	9.9549-1
NA2SO4(L)	9.9346-1	0.000000	9.9528-1	0.000000
NA2V2O6(L)	6.4598-3	4.3220-3	4.6882-3	2.9960-3
NA4V2O7(S)	4.7736-5	2.0107-8	2.1144-6	1.2283-9
NA6V2O8(S)	1.7180-9	0.000 0	4.644-12	0.000 0
V2O3(S)	3.646-12	2.859-12	6.195-12	3.214-12
V2O5(L)	1.1677-6	1.9201-4	1.3886-5	1.5104-3
M, MOL WT	142.70	142.48	142.51	142.40
PHASE FRACTION	1.8898-7	2.7249-7	2.6147-7	2.7295-7

PURE SPECIES PHASE FRACTIONS (IF ANY)

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-11 FOR ALL ASSIGNED CONDITI

SOLUTION 1

C	CH	CH2	CH2O	CH2O2	CH3	CH2OH	CH3O	CH4	CH
CN	CN2	CNN	COS	CS	CS2	C2	C2H	C2H2	C2
C2H4	C2H4O2	C2H4O4	C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3	C2N	C2
C2O	C3	C3H6O	N-C3H7	I-C3H7	C3H8	I-C3H7OH	C3O2	C4	C4
N-C4H10	I-C4H10	C4N2	C5	C6H5	C6H5O	C6H6	C6H5OH	C7H8	C8
N-C8H18	I-C8H18	O-C12H9	C12H10	HCN	HCO	HNCO	H2N2	H2S	N
NCO	NH	NH2	NH3	NO3	N2H4	N2O4	N2O5	N3	NA
NAH	NAO	NA2	NA2C2N2	NA2O	NA2O2H2	S	SH	SN	SO
S2	S2O	S8	V	VN	VO	VO2			

SOLUTION 2

NAOH(A)	NA2O(A)	NA2O(L)	NA2SO4(IV)	NA2V2O6(S)	NA6V2O8(L)	V2O3(L)	V2O5(S)	
PURE SPECIES								
C(GR)	C7H8(L)	C8H18(L)	H2O(S)	H2O(L)	H2SO4(L)	VN(S)	N2H6SO4(S)	NA(S)
NACN(S)	NACN(L)	NAO2(S)	NA2CO3(1)	NA2CO3(2)	NA2CO3(L)	NA2O2(A)	NA2O2(B)	NA2S(1)
NA2S(L)	S(S)	S(L)	V(S)	V(L)	NAV3O8(S)	NA2V12O31(S)	NA2V12O31(L)	VO(S)
VO2(S)	VO2(S)	VO2(L)						

H 2.000000 0 1.000000 0.000000 0.000000 00 0.000000 0.01000000 0.00 G 298.150 0 0.00000

CASE NO. 8701 122 0.1% SULFUR, 0.1 NA, 1.0 V PPM TIME = 0.609 SEC

P, ATM	1.0000	1.0000	7.0000	7.0000	10.000	10.000	15.000	15.000
T, DEG K	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0
SOLUTION 1								
AR	8.8009-3	8.8009-3	8.8009-3	8.8010-3	8.8009-3	8.8010-3	8.8009-3	8.8010-3
CO	3.0930-9	9.522-12	1.1690-9	3.599-12	9.783-10	3.011-12	7.988-10	2.459-12
CO2	9.0818-2	9.0819-2	9.0819-2	9.0819-2	9.0819-2	9.0819-2	9.0819-2	9.0820-2
H	5.870-12	4.831-15	1.364-12	1.123-15	1.044-12	8.591-16	7.702-13	6.338-16
HNO	1.515-12	1.651-14	2.464-12	2.686-14	2.694-12	2.936-14	2.981-12	3.249-14
HNO2	4.1223-9	1.6068-9	1.7740-8	6.9143-9	2.3180-8	9.0349-9	3.1418-8	1.2246-8
HNO3	1.207-11	1.511-11	1.374-10	1.720-10	2.146-10	2.686-10	3.562-10	4.459-10
HO2	1.1960-8	9.707-10	1.9450-8	1.5790-9	2.1260-8	1.7260-9	2.3530-8	1.9100-9
H2	2.6110-9	1.616-11	9.868-10	6.106-12	8.256-10	5.109-12	6.741-10	4.172-12
H2O	9.6876-2	9.6877-2	9.6876-2	9.6878-2	9.6877-2	9.6878-2	9.6877-2	9.6878-2
H2O2	4.817-10	5.487-11	1.2740-9	1.452-10	1.5230-9	1.735-10	1.8650-9	2.125-10
H2SO4	2.729-10	8.2480-9	4.4810-9	9.3600-8	7.3880-9	1.4240-7	1.2960-8	2.2720-7
NO	9.4506-5	1.4826-5	9.4503-5	1.4825-5	9.4503-5	1.4825-5	9.4502-5	1.4825-5
NO2	1.0024-6	5.2000-7	2.6521-6	1.3757-6	3.1698-6	1.6442-6	3.8821-6	2.0137-6
NO3	1.257-13	2.780-14	8.801-13	1.946-13	1.257-12	2.779-13	1.886-12	4.169-13
N2	7.3702-1	7.3707-1	7.3702-1	7.3707-1	7.3702-1	7.3707-1	7.3702-1	7.3707-1
N2O	5.6021-9	1.0097-9	1.4821-8	2.6714-9	1.7715-8	3.1929-9	2.1696-8	3.9105-9
NAOH	2.446-10	5.007-13	9.383-11	1.455-13	7.850-11	1.098-13	6.400-11	7.789-14
NA2SO4	3.217-12	1.323-12	7.774-12	1.268-12	8.972-12	1.097-12	1.046-11	8.821-13
O	3.4960-9	1.968-11	1.3210-9	7.437-12	1.1060-9	6.222-12	9.027-10	5.080-12
OH	1.5470-6	5.5769-8	9.5107-7	3.4286-8	8.6994-7	3.1361-8	7.8607-7	2.8337-8
O2	6.6346-2	6.6381-2	6.6343-2	6.6376-2	6.6342-2	6.6375-2	6.6340-2	6.6374-2
O3	1.885-12	9.975-14	4.988-12	2.639-13	5.962-12	3.154-13	7.302-12	3.863-13
SO2	3.6745-5	2.4617-5	3.2582-5	1.5084-5	3.1462-5	1.3438-5	3.0040-5	1.1674-5
SO3	3.0899-6	1.5210-5	7.2487-6	2.4657-5	8.3659-6	2.6254-5	9.7828-6	2.7933-5
M, MOL WT	28.869	28.869	28.869	28.869	28.869	28.869	28.869	28.869
PHASE FRACTION	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0
SOLUTION 2								
NAOH(L)	2.0265-7	2.1963-8	5.4418-7	4.4681-8	6.5040-7	4.8144-8	7.9530-7	5.1248-8
NA2SO3(L)	0.000 0	0.000 0	1.120-12	0.000 0	1.545-12	0.000 0	2.205-12	0.000 0
NA2SO4(I)	0.000000	1.1804-2	0.000000	7.9189-2	0.000000	9.7896-2	0.000000	1.1802-1
NA2SO4(L)	4.8431-5	0.000000	8.1926-4	0.000000	1.3507-3	0.000000	2.3616-3	0.000000
NA2V206(L)	2.1132-1	2.0706-1	2.1614-1	2.1475-1	2.1602-1	1.0191-1	2.1525-1	7.7409-2
NA4V207(S)	7.5642-8	1.1344-8	7.9696-8	4.0408-9	7.9648-8	2.6829-9	7.9112-8	1.5394-9
V203(S)	2.4630-6	1.1630-8	3.4930-7	1.6940-9	2.4440-7	1.1920-9	1.6290-7	7.989-10
V205(L)	7.8863-1	7.8114-1	7.8304-1	7.9606-1	7.8263-1	8.0019-1	7.8238-1	8.0457-1
M, MOL WT	194.98	194.24	195.24	186.46	195.21	184.30	195.13	181.98
PHASE FRACTION	1.2301-8	1.2447-8	1.2310-8	1.3358-8	1.2317-8	1.3635-8	1.2329-8	1.3946-8

PURE SPECIES PHASE FRACTIONS (IF ANY)

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-11 FOR ALL ASSIGNED CONDITI

SOLUTION 1

C	CH	CH2	CH2O	CH2O2	CH3	CH2OH	CH3O	CH4	CH
CN	CN2	CNN	COS	CS	CS2	C2	C2H	C2H2	C2
C2H4	C2H4O2	C2H4O4	C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3	C2N	C2
C2O	C3	C3H6O	N-C3H7	I-C3H7	C3H8	1-C3H7OH	C3O2	C4	C4
N-C4H10	I-C4H10	C4N2	C5	C6H5	C6H5O	C6H6	C6H5OH	C7H8	C8
N-C8H18	I-C8H18	O-C12H9	C12H10	HCN	HCO	HNCO	H2N2	H2S	N
NCO	NH	NH2	NH3	N2H4	N2O4	N2O5	N3	NA	NA
NAH	NAO	NA2	NA2C2N2	NA2O	NA2O2H2	S	SH	SN	SO
S2	S2O	S8	V	VN	VO	VO2			

SOLUTION 2

NAOH(A)	NA2O(C)	NA2O(A)	NA2O(L)	NA2SO3(S)	NA2SO4(IV)	NA2V206(S)	NA6V208(S)	NA6V208(L)	V2
V205(S)									

PURE SPECIES

C(GR)	C7H8(L)	C8H18(L)	H2O(S)	H2O(L)	H2SO4(L)	VN(S)	N2H6SO4(S)	NA(S)	NA
NACN(S)	NACN(L)	NAO2(S)	NA2CO3(1)	NA2CO3(2)	NA2CO3(L)	NA2O2(A)	NA2O2(B)	NA2S(1)	NA
NA2S(L)	S(S)	S(L)	V(S)	V(L)	NAV3O8(S)	NA2V12O31(S)	NA2V12O31(L)	VO(S)	VO
VO2(S)	VO2(S)	VO2(L)							

CASE NO. 8701 222 0.1% SULFUR, 1.0 NA, 1.0 V PPM TIME = 0.749 SEC

P, ATM	1.0000	1.0000	7.0000	7.0000	10.000	10.000	15.000	15.000
T, DEG K	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0
SOLUTION 1								
AR	8.8009-3	8.8009-3	8.8009-3	8.8010-3	8.8009-3	8.8010-3	8.8009-3	8.8010-3
CO	3.0930-9	9.522-12	1.1690-9	3.599-12	9.783-10	3.011-12	7.988-10	2.459-12
CO2	9.0818-2	9.0819-2	9.0819-2	9.0819-2	9.0819-2	9.0819-2	9.0819-2	9.0819-2
H	5.970-12	4.831-15	1.364-12	1.123-15	1.044-12	8.591-16	7.702-13	6.338-16
HNO	1.515-12	1.651-14	2.464-12	2.686-14	2.694-12	2.936-14	2.981-12	3.249-14
HNO2	4.1223-9	1.6068-9	1.7740-8	6.9144-9	2.3180-8	9.0349-9	3.1418-8	1.2246-8
HNO3	1.207-11	1.511-11	1.374-10	1.720-10	2.146-10	2.686-10	3.562-10	4.459-10
HO2	1.1960-8	9.707-10	1.9450-8	1.5790-9	2.1260-8	1.7260-9	2.3530-8	1.9100-9
H2	2.6110-9	1.616-11	9.868-10	6.106-12	8.256-10	5.109-12	6.741-10	4.172-12
H2O	9.6876-2	9.6877-2	9.6876-2	9.6878-2	9.6876-2	9.6878-2	9.6877-2	9.6878-2
H2O2	4.817-10	5.487-11	1.2740-9	1.452-10	1.5230-9	1.735-10	1.8650-9	2.125-10
H2SO4	2.728-10	8.2450-9	4.4790-9	9.3550-8	7.3850-9	1.4230-7	1.2950-8	2.2710-7
NO	9.4506-5	1.4826-5	9.4504-5	1.4825-5	9.4503-5	1.4825-5	9.4502-5	1.4825-5
NO2	1.0024-6	5.2000-7	2.6521-6	1.3757-6	3.1698-6	1.6442-6	3.8821-6	2.0137-6
NO3	1.257-13	2.780-14	8.801-13	1.946-13	1.257-12	2.779-13	1.886-12	4.169-13
N2	7.3702-1	7.3707-1	7.3702-1	7.3707-1	7.3702-1	7.3707-1	7.3702-1	7.3707-1
N2O	5.6021-9	1.0097-9	1.4821-8	2.6714-9	1.7715-8	3.1929-9	2.1696-8	3.9105-9
NA	1.527-12	1.104-17	6.554-14	3.033-19	3.391-14	1.592-19	1.586-14	7.671-20
NAOH	1.1810-8	3.456-12	2.1800-9	4.087-13	1.4740-9	2.803-13	9.344-10	1.830-13
NA2SO4	7.4950-9	6.302-11	4.1960-9	9.999-12	3.1630-9	7.151-12	2.2290-9	4.868-12
O	3.4960-9	1.968-11	1.3210-9	7.437-12	1.1060-9	6.222-12	9.027-10	5.080-12
OH	1.5470-6	5.5769-8	9.5107-7	3.4286-8	8.6994-7	3.1361-8	7.8607-7	2.8337-8
O2	6.6346-2	6.6381-2	6.6343-2	6.6376-2	6.6342-2	6.6375-2	6.6340-2	6.6374-2
O3	1.885-12	9.975-14	4.988-12	2.639-13	5.962-12	3.154-13	7.302-12	3.863-13
SO2	3.6737-5	2.4608-5	3.2571-5	1.5077-5	3.1451-5	1.3431-5	3.0029-5	1.1668-5
SO3	3.0892-6	1.5204-5	7.2462-6	2.4645-5	8.3629-6	2.6241-5	9.7792-6	2.7918-5
M, MOL WT	28.869	28.869	28.869	28.869	28.869	28.869	28.869	28.869
PHASE FRACTION	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0
SOLUTION 2								
NAOH(L)	9.7828-6	1.5160-7	1.2644-5	1.2549-7	1.2213-5	1.2293-7	1.1612-5	1.2043-7
NA2SO3(S)	0.000 0	5.126-12	0.000 0	2.152-12	0.000 0	1.839-12	0.000 0	1.534-12
NA2SO3(L)	4.081-10	0.000 0	6.044-10	0.000 0	5.446-10	0.000 0	4.700-10	0.000 0
NA2SO4(I)	0.000000	5.6216-1	0.000000	6.2437-1	0.000000	6.3789-1	0.000000	6.5139-1
NA2SO4(L)	1.1284-1	0.000000	4.4214-1	0.000000	4.7611-1	0.000000	5.0330-1	0.000000
NA2V2O6(L)	8.8500-1	4.0571-1	5.5402-1	2.0765-1	5.1848-1	1.6427-1	4.8832-1	1.2096-1
NA4V2O7(S)	7.3824-4	1.0591-6	1.1029-4	5.3058-8	6.7410-5	2.8192-8	3.8263-5	1.3282-8
NA6V2O8(S)	2.9990-9	0.000 0	1.069-10	0.000 0	4.269-11	0.000 0	1.460-11	0.000 0
V2O3(S)	4.4250-9	4.784-10	1.6590-9	3.574-10	1.6640-9	2.947-10	1.7330-9	2.261-10
V2O5(L)	1.4172-3	3.2125-2	3.7178-3	1.6797-1	5.3272-3	1.9784-1	8.3250-3	2.2766-1
M, MOL WT	232.33	184.63	198.61	169.87	195.05	166.65	192.10	163.42
PHASE FRACTION	1.3865-8	2.8093-8	2.2050-8	3.2746-8	2.3479-8	3.3969-8	2.4765-8	3.5284-8

PURE SPECIES PHASE FRACTIONS (IF ANY)

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-11 FOR ALL ASSIGNED CONDITI

SOLUTION 1

C	CH	CH2	CH2O	CH2O2	CH3	CH2OH	CH3O	CH4
CN	CN2	CNN	COS	CS	CS2	C2	C2H	C2H2
C2H4	C2H4O2	C2H4O4	C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3	C2N
C2O	C3	C3H6O	N-C3H7	I-C3H7	C3H8	1-C3H7OH	C3O2	C4
N-C4H10	I-C4H10	C4N2	C5	C6H5	C6H5O	C6H6	C6H5OH	C7H8
N-C8H18	I-C8H18	O-C12H9	C12H10	HCN	HCO	HNCO	H2N2	H2S
NCO	NH	NH2	NH3	N2H4	N2O4	N2O5	N3	NACN
NAO	NA2	NA2C2N2	NA2O	NA2O2H2	S	SH	SN	SO
S2O	S8	V	VN	VO	VO2			

SOLUTION 2

NAOH(A)	NA2O(C)	NA2O(A)	NA2O(L)	NA2SO4(IV)	NA2V2O6(S)	NA6V2O8(L)	V2O3(L)	V2O5(S)

PURE SPECIES

C(GR)	C7H8(L)	C8H18(L)	H2O(S)	H2O(L)	H2SO4(L)	VN(S)	N2H6SO4(S)	NA(S)	NA
NACN(S)	NACN(L)	NAO2(S)	NA2CO3(1)	NA2CO3(2)	NA2CO3(L)	NA2O2(A)	NA2O2(B)	NA2S(1)	NA
NA2S(L)	S(S)	S(L)	V(S)	V(L)	NAV3O8(S)	NA2V12O31(S)	NA2V12O31(L)	VO(S)	VO
VO2(S)	VO2(S)	VO2(L)						

CASE NO. 8701 322 0.1% SULFUR, 10 NA, 1.0 V PPM singular matrix, iteration 30 variable 7

P, ATM	1.0000	1.0000
T, DEG K	1172.0	977.0
SOLUTION 1		
AR	8.8009-3	8.8010-3
CO	3.0930-9	9.522-12
CO2	9.0817-2	9.0818-2
H	5.870-12	4.831-15
HNO	1.515-12	1.651-14
HNO2	4.1223-9	1.6068-9
HNO3	1.207-11	1.511-11
HO2	1.1960-8	9.707-10
H2	2.6110-9	1.616-11
H2O	9.6875-2	9.6876-2
H2O2	4.817-10	5.487-11
H2SO4	2.712-10	8.1940-9
NO	9.4507-5	1.4826-5
NO2	1.0025-6	5.2001-7
N2	7.3702-1	7.3707-1
N2O	5.6021-9	1.0097-9
NA	4.413-12	1.443-17
NAOH	3.4110-8	4.519-12
NA2SO4	6.2190-8	1.071-10
O	3.4960-9	1.968-11
OH	1.5470-6	5.5769-8
O2	6.6347-2	6.6382-2
O3	1.886-12	9.975-14
SO2	3.6521-5	2.4456-5
SO3	3.0710-6	1.5110-5
M, MOL WT	28.869	28.869
PHASE FRACTION	1.0000 0	1.0000 0
SOLUTION 2		
NAOH(L)	2.8263-5	1.9820-7
NA2O(C)	1.644-12	0.000 0
NA2SO3(S)	0.000 0	8.707-12
NA2SO3(L)	3.3865-9	0.000000
NA2SO4(I)	0.000000	9.5494-1
NA2SO4(L)	9.3631-1	0.000000
NA2V2O6(L)	6.3207-2	4.3063-2
NA4V2O7(S)	4.4009-4	1.9213-7
NA6V2O8(S)	1.4925-8	0.000000
V2O3(S)	3.787-11	2.971-11
V2O5(L)	1.2127-5	1.9949-3
M, MOL WT	148.54	146.50
PHASE FRACTION	1.9322-7	2.7299-7

PURE SPECIES PHASE FRACTIONS (IF ANY)

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-11 FOR ALL ASSIGNED CONDITI

SOLUTION 1

C	CH	CH2	CH2O	CH2O2	CH3	CH2OH	CH3O	CH4	CH
CN	CN2	CNN	COS	CS	CS2	C2	C2H	C2H2	C2
C2H4	C2H4O2	C2H4O4	C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3	C2N	C2
C2O	C3	C3H6O	N-C3H7	I-C3H7	C3H8	1-C3H7OH	C3O2	C4	C4
N-C4H10	I-C4H10	C4N2	C5	C6H5	C6H5O	C6H6	C6H5OH	C7H8	C8
N-C8H18	I-C8H18	O-C12H9	C12H10	HCN	HCO	HNCO	H2N2	H2S	N
NCO	NH	NH2	NH3	NO3	N2H4	N2O4	N2O5	N3	NA
NAH	NAO	NA2	NA2C2N2	NA2O	NA2O2H2	S	SH	SN	SO
S2	S2O	S8	V	VN	VO	VO2			

SOLUTION 2

NAOH(A)	NA2O(A)	NA2O(L)	NA2SO4(IV)	NA2V2O6(S)	NA6V2O8(L)	V2O3(L)	V2O5(S)		
PURE SPECIES									
C(GR)	C7H8(L)	C8H18(L)	H2O(S)	H2O(L)	H2SO4(L)	VN(S)	N2H6SO4(S)	NA(S)	NA
NACN(S)	NACN(L)	NAO2(S)	NA2CO3(I)	NA2CO3(2)	NA2CO3(L)	NA2O2(A)	NA2O2(B)	NA2S(1)	NA
NA2S(L)	S(S)	S(L)	V(S)	V(L)	NAV3O8(S)	NA2V12O31(S)	NA2V12O31(L)	VO(S)	VO
VO2(S)	VO2(S)	VO2(L)							

CASE NO. 8701 123 0.1% SULFUR, 0.1 NA, 10 V PPM TIME = 0.598 SEC

P, ATM		1.0000	1.0000	7.0000	7.0000	10.000	10.000	15.000	15.000
T, DEG K		1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0
SOLUTION 1									
AR		8.8009-3	8.8010-3	8.8009-3	8.8010-3	8.8009-3	8.8010-3	8.8009-3	8.8010-3
CO		3.0930-9	9.522-12	1.1690-9	3.599-12	9.783-10	3.011-12	7.988-10	2.459-12
CO2		9.0818-2	9.0818-2	9.0818-2	9.0819-2	9.0818-2	9.0819-2	9.0818-2	9.0819-2
H		5.870-12	4.831-15	1.364-12	1.123-15	1.044-12	8.591-16	7.702-13	6.338-16
HNO		1.515-12	1.651-14	2.464-12	2.686-14	2.694-12	2.936-14	2.981-12	3.249-14
HNO2		4.1223-9	1.6068-9	1.7740-8	6.9144-9	2.3181-8	9.0350-9	3.1419-8	1.2246-8
HNO3		1.207-11	1.511-11	1.374-10	1.720-10	2.146-10	2.686-10	3.562-10	4.459-10
HO2		1.1960-8	9.707-10	1.9450-8	1.5790-9	2.1260-8	1.7260-9	2.3530-8	1.9100-9
H2		2.6110-9	1.616-11	9.868-10	6.106-12	8.256-10	5.109-12	6.741-10	4.171-12
H2O		9.6875-2	9.6876-2	9.6876-2	9.6877-2	9.6876-2	9.6877-2	9.6876-2	9.6877-2
H2O2		4.817-10	5.487-11	1.2740-9	1.452-10	1.5230-9	1.735-10	1.8650-9	2.125-10
H2SO4		2.729-10	8.2480-9	4.4810-9	9.3600-8	7.3880-9	1.4240-7	1.2960-8	2.2720-7
NO		9.4507-5	1.4826-5	9.4504-5	1.4826-5	9.4503-5	1.4825-5	9.4503-5	1.4825-5
NO2		1.0025-6	5.2001-7	2.6521-6	1.3757-6	3.1698-6	1.6443-6	3.8822-6	2.0138-6
NO3		1.257-13	2.780-14	8.801-13	1.946-13	1.257-12	2.779-13	1.886-12	4.169-13
N2		7.3702-1	7.3707-1	7.3702-1	7.3707-1	7.3702-1	7.3707-1	7.3702-1	7.3707-1
N2O		5.6021-9	1.0097-9	1.4821-8	2.6714-9	1.7715-8	3.1930-9	2.1696-8	3.9105-9
NAOH		7.065-11	1.431-13	2.678-11	4.476-14	2.239-11	3.447-14	1.825-11	2.502-14
O		3.4960-9	1.968-11	1.3210-9	7.437-12	1.1060-9	6.222-12	9.027-10	5.080-12
OH		1.5470-6	5.5769-8	9.5107-7	3.4286-8	8.6994-7	3.1361-8	7.8607-7	2.8337-8
O2		6.6347-2	6.6382-2	6.6344-2	6.6377-2	6.6343-2	6.6376-2	6.6341-2	6.6375-2
O3		1.886-12	9.975-14	4.988-12	2.639-13	5.962-12	3.154-13	7.302-12	3.863-13
SO2		3.6745-5	2.4617-5	3.2582-5	1.5084-5	3.1462-5	1.3438-5	3.0040-5	1.1674-5
SO3		3.0899-6	1.5210-5	7.2487-6	2.4657-5	8.3659-6	2.6254-5	9.7828-6	2.7933-5
M, MOL WT		28.869	28.869	28.869	28.869	28.869	28.869	28.869	28.869
PHASE FRACTION		1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0
SOLUTION 2									
NAOH(L)		5.8534-8	6.2772-9	1.5529-7	1.3743-8	1.8549-7	1.5121-8	2.2683-7	1.6462-8
NA2SO4(I)		0.000000	9.6415-4	0.000000	7.4920-3	0.000000	9.6567-3	0.000000	1.2178-2
NA2SO4(L)		4.0406-6	0.000000	6.6713-5	0.000000	1.0986-4	0.000000	1.9212-4	0.000000
NA2V2O6(L)		2.1867-2	2.1173-2	2.1981-2	1.4500-2	2.1955-2	1.2288-2	2.1888-2	9.7104-3
NA4V2O7(S)		6.530-10	9.475-11	6.600-10	4.444-11	6.584-10	3.191-11	6.544-10	1.992-11
V2O3(S)		3.0540-6	1.4560-8	4.3630-7	2.0810-9	3.0540-7	1.4570-9	2.0360-7	9.712-10
V2O5(L)		9.7813-1	9.7786-1	9.7795-1	9.7801-1	9.7794-1	9.7806-1	9.7792-1	9.7811-1
M, MOL WT		183.24	183.15	183.24	182.48	183.24	182.26	183.23	182.00
PHASE FRACTION		1.2300-7	1.2312-7	1.2301-7	1.2393-7	1.2302-7	1.2420-7	1.2303-7	1.2452-7

PURE SPECIES PHASE FRACTIONS (IF ANY)

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-11 FOR ALL ASSIGNED CONDITI

SOLUTION 1

C	CH	CH2	CH2O	CH2O2	CH3	CH2OH	CH3O	CH4	CH
CN	CN2	CNN	COS	CS	CS2	C2	C2H	C2H2	C2
C2H4	C2H4O2	C2H4O4	C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3	C2N	C2
C2O	C3	C3H6O	N-C3H7	I-C3H7	C3H8	1-C3H7OH	C3O2	C4	C4
N-C4H10	I-C4H10	C4N2	C5	C6H5	C6H5O	C6H6	C6H5OH	C7H8	C8
N-C8H18	I-C8H18	O-C12H9	C12H10	HCN	HCO	HNCO	H2N2	H2S	N
NCO	NH	NH2	NH3	N2H4	N2O4	N2O5	N3	NA	NA
NAH	NAO	NA2	NA2C2N2	NA2O	NA2O2H2	NA2SO4	S	SH	SN
SO	S2	S2O	S8	V	VN	VO	VO2		

SOLUTION 2

NAOH(A)	NA2O(C)	NA2O(A)	NA2O(L)	NA2SO3(S)	NA2SO3(L)	NA2SO4(IV)	NA2V2O6(S)	NA6V2O8(S)	NA
V2O3(L)	V2O5(S)								

PURE SPECIES

C(GR)	C7H8(L)	C8H18(L)	H2O(S)	H2O(L)	H2SO4(L)	VN(S)	N2H6SO4(S)	NA(S)	NA
NAOH(S)	NAOH(L)	NAO2(S)	NA2CO3(1)	NA2CO3(2)	NA2CO3(L)	NA2O2(A)	NA2O2(B)	NA2S(1)	NA

NA2S(L)	S(S)	S(L)	V(S)	V(L)	NAV3O8(S)	NA2V12O31(S)	NA2V12O31(L)	VO(S)	VO
VO2(S)	VO2(S)	VO2(L)							

CASE NO. 8701 223 0.1% SULFUR, 1.0 NA, 10 V PPM TIME = 0.603 SEC

P, ATM	1.0000	1.0000	7.0000	7.0000	10.000	10.000	15.000	15.000
T, DEG K	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0
SOLUTION 1								
AR	8.8009-3	8.8010-3	8.8009-3	8.8010-3	8.8009-3	8.8010-3	8.8009-3	8.8010-3
CO	3.0930-9	9.522-12	1.1690-9	3.599-12	9.783-10	3.011-12	7.988-10	2.459-12
CO2	9.0817-2	9.0818-2	9.0818-2	9.0819-2	9.0818-2	9.0819-2	9.0818-2	9.0819-2
H	5.870-12	4.831-15	1.364-12	1.123-15	1.044-12	8.591-16	7.702-13	6.338-16
HNO	1.515-12	1.651-14	2.464-12	2.686-14	2.694-12	2.936-14	2.981-12	3.249-14
HNO2	4.1223-9	1.6068-9	1.7740-8	6.9144-9	2.3181-8	9.0350-9	3.1419-8	1.2246-8
HNO3	1.207-11	1.511-11	1.374-10	1.720-10	2.146-10	2.686-10	3.562-10	4.459-10
HO2	1.1960-8	9.707-10	1.9450-8	1.5790-9	2.1260-8	1.7260-9	2.3330-8	1.9100-9
H2	2.6110-9	1.616-11	9.868-10	6.106-12	8.256-10	5.109-12	6.741-10	4.171-12
H2O	9.6875-2	9.6876-2	9.6876-2	9.6877-2	9.6876-2	9.6877-2	9.6876-2	9.6877-2
H2O2	4.817-10	5.487-11	1.2740-9	1.452-10	1.5230-9	1.735-10	1.8650-9	2.125-10
H2SO4	2.729-10	8.2480-9	4.4810-9	9.3580-8	7.3880-9	1.4230-7	1.2960-8	2.2710-7
NO	9.4507-5	1.4826-5	9.4504-5	1.4826-5	9.4504-5	1.4825-5	9.4503-5	1.4825-5
NO2	1.0025-6	5.2001-7	2.6521-6	1.3757-6	3.1698-6	1.6443-6	3.8822-6	2.0138-6
NO3	1.257-13	2.780-14	8.801-13	1.946-13	1.257-12	2.779-13	1.886-12	4.169-13
N2	7.3702-1	7.3707-1	7.3702-1	7.3707-1	7.3702-1	7.3707-1	7.3702-1	7.3707-1
N2O	5.6021-9	1.0097-9	1.4821-8	2.6714-9	1.7715-8	3.1930-9	2.1696-8	3.9105-9
NAOH	2.513-10	5.009-13	9.493-11	1.456-13	7.931-11	1.098-13	6.457-11	7.790-14
NA2SO4	3.396-12	1.324-12	7.957-12	1.269-12	9.158-12	1.098-12	1.065-11	8.820-13
O	3.4960-9	1.968-11	1.3210-9	7.437-12	1.1060-9	6.222-12	9.027-10	5.080-12
OH	1.5470-6	5.5769-8	9.5107-7	3.4286-8	8.6994-7	3.1361-8	7.8607-7	2.8337-8
O2	6.6347-2	6.6382-2	6.6344-2	6.6377-2	6.6343-2	6.6376-2	6.6341-2	6.6375-2
O3	1.886-12	9.975-14	4.988-12	2.639-13	5.962-12	3.154-13	7.302-12	3.863-13
SO2	3.6745-5	2.4616-5	3.2582-5	1.5080-5	3.1462-5	1.3434-5	3.0039-5	1.1669-5
SO3	3.0899-6	1.5209-5	7.2487-6	2.4651-5	8.3659-6	2.6246-5	9.7827-6	2.7923-5
M, MOL WT	28.869	28.869	28.869	28.869	28.869	28.869	28.869	28.869
PHASE FRACTION	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0
SOLUTION 2								
NAOH(L)	2.0820-7	2.1969-8	5.5055-7	4.4693-8	6.5710-7	4.8157-8	8.0248-7	5.1255-8
NA2SO3(L)	0.000 0	0.000 0	1.146-12	0.000 0	1.577-12	0.000 0	2.245-12	0.000 0
NA2SO4(I)	0.000000	1.1810-2	0.000000	7.9213-2	0.000000	9.7918-2	0.000000	1.1801-1
NA2SO4(L)	5.1122-5	0.000000	8.3857-4	0.000000	1.3787-3	0.000000	2.4044-3	0.000000
NA2V206(L)	2.2047-1	2.0715-1	2.2011-1	1.2481-1	2.1950-1	1.0196-1	2.1830-1	7.7428-2
NA4V207(S)	8.3303-8	1.1355-8	8.3073-8	4.0449-9	8.2609-8	2.6855-9	8.1686-8	1.5401-9
V203(S)	2.4340-6	1.1630-8	3.4750-7	1.6940-9	2.4330-7	1.1920-9	1.6220-7	7.989-10
V205(L)	7.7947-1	7.8104-1	7.7905-1	7.9598-1	7.7912-1	8.0012-1	7.7930-1	8.0457-1
M, MOL WT	195.54	194.25	195.49	186.46	195.43	184.30	195.31	181.98
PHASE FRACTION	1.2301-7	1.2447-7	1.2311-7	1.3358-7	1.2317-7	1.3635-7	1.2330-7	1.3946-7

PURE SPECIES PHASE FRACTIONS (IF ANY)

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-11 FOR ALL ASSIGNED CONDITI

SOLUTION 1

C	CH	CH2	CH2O	CH2O2	CH3	CH2OH	CH3O	CH4
CH	CN	CN2	CNN	COS	CS	CS2	C2	C2H
C2H2	C2H4O2	C2H4O4	C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3	C2N
C2O	C3	C3H6O	N-C3H7	I-C3H7	C3H8	1-C3H7OH	C3O2	C4
N-C4H10	I-C4H10	C4N2	C5	C6H5	C6H5O	C6H6	C6H5OH	C7H8
N-C8H18	I-C8H18	O-C12H9	C12H10	HCN	HCO	HNCO	H2N2	H2S
NCO	NH	NH2	NH3	N2H4	N2O4	N2O5	N3	NA
NAH	NAO	NA2	NA2C2N2	NA2O	NA2O2H2	S	SH	SN
S2	S2O	S8	V	VN	VO	VO2		

SOLUTION 2

NAOH(A)	NA2O(C)	NA2O(A)	NA2O(L)	NA2SO3(S)	NA2SO4(IV)	NA2V2O6(S)	NA6V2O8(S)	NA6V2O8(L)
V2	V2O5(S)							

PURE SPECIES

C(GR)	C7H8(L)	C8H18(L)	H2O(S)	H2O(L)	H2SO4(L)	VN(S)	N2H6SO4(S)	NA(S)
NA	NACN(S)	NACN(L)	NAO2(S)	NA2CO3(1)	NA2CO3(2)	NA2CO3(L)	NA2O2(A)	NA2O2(B)
NA2S(1)	NA	NA2S(L)	S(S)	S(L)	V(S)	V(L)	NAV3O8(S)	NA2V12O31(S)
NA2V12O31(L)	VO(S)	VO	VO2(S)	VO2(S)	VO2(L)			

CASE NO. 8701 323 0.1% SULFUR, 10 NA, 10 V PPM Osingular matrix, iteration 30 variable 1

P, ATM	1.0000	1.0000
T, DEG K	1172.0	977.0
SOLUTION 1		
AR	8.8009-3	8.8010-3
CO	3.0930-9	9.521-12
CO2	9.0817-2	9.0817-2
H	5.870-12	4.831-15
HNO	1.515-12	1.651-14
HNO2	4.1224-9	1.6068-9
HNO3	1.207-11	1.511-11
HO2	1.1960-8	9.708-10
H2	2.6110-9	1.615-11
H2O	9.6874-2	9.6876-2
H2O2	4.817-10	5.487-11
H2SO4	2.719-10	8.2150-9
NO	9.4507-5	1.4826-5
NO2	1.0025-6	5.2002-7
N2	7.3702-1	7.3707-1
N2O	5.6022-9	1.0098-9
NA	3.102-12	1.107-17
NAOH	2.3980-8	3.465-12
NA2SO4	3.0800-8	6.312-11
O	3.4960-9	1.968-11
OH	1.5470-6	5.5769-8
O2	6.6348-2	6.6383-2
O3	1.886-12	9.975-14
SO2	3.6618-5	2.4519-5
SO3	3.0792-6	1.5149-5
M, MOL WT	28.869	28.869
PHASE FRACTION	1.0000 0	1.0000 0
SOLUTION 2		
NAOH(L)	1.9865-5	1.5199-7
NA2SO3(S)	0.000 0	5.133-12
NA2SO3(L)	1.6773-9	0.000000
NA2SO4(I)	0.000000	5.6300-1
NA2SO4(L)	4.6376-1	0.000000
NA2V2O6(L)	5.3418-1	4.0509-1
NA4V2O7(S)	1.8373-3	1.0628-6
NA6V2O8(S)	3.0778-8	0.000000
V2O3(S)	6.478-10	4.752-10
V2O5(L)	2.0747-4	3.1912-2
M, MOL WT	196.74	184.56
PHASE FRACTION	2.2938-7	2.8147-7

PURE SPECIES PHASE FRACTIONS (IF ANY)

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-11 FOR ALL ASSIGNED CONDITI

SOLUTION 1

C	CH	CH2	CH2O	CH2O2	CH3	CH2OH	CH3O	CH4	CH
CN	CN2	CNN	COS	CS	CS2	C2	C2H	C2H2	C2
C2H4	C2H4O2	C2H4O4	C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3	C2N	C2
C2O	C3	C3H6O	N-C3H7	I-C3H7	C3H8	1-C3H7OH	C3O2	C4	C4
N-C4H10	I-C4H10	C4N2	C5	C6H5	C6H5O	C6H6	C6H5OH	C7H8	C8
N-C8H18	I-C8H18	O-C12H9	C12H10	HCN	HCO	HNCO	H2N2	H2S	N
NCO	NH	NH2	NH3	NO3	N2H4	N2O4	N2O5	N3	NA
NAH	NAO	NA2	NA2C2N2	NA2O	NA2O2H2	S	SH	SN	SO
S2	S2O	S8	V	VN	VO	VO2			

SOLUTION 2

NAOH(A)	NA2O(C)	NA2O(A)	NA2O(L)	NA2SO4(IV)	NA2V2O6(S)	NA6V2O8(L)	V2O3(L)	V2O5(S)

PURE SPECIES

C(GR)	C7H8(L)	C8H18(L)	H2O(S)	H2O(L)	H2SO4(L)	VN(S)	N2H6SO4(S)	NA(S)
NACN(S)	NACN(L)	NAO2(S)	NA2CO3(1)	NA2CO3(2)	NA2CO3(L)	NA2O2(A)	NA2O2(B)	NA2S(1)
NA2S(L)	S(S)	S(L)	V(S)	V(L)	NAV3O8(S)	NA2V12O31(S)	NA2V12O31(L)	VO(S)
VO2(S)	VO2(S)	VO2(L)						

STOP

VISNVHP V-NA SYSTEMS CORROSION THEORY 01/87

SOLN 1 GASES

SOLN 2 V2O5(L) V2O3(L) V2O4(L)
SOLN 2 NA2SO3(L) NA2SO4(L) NAOH(L)
SOLN 2 NA2O(L) NA2V2O6(S) NA4V2O7(S) NA6V2O8(S)

CASE NO. 8701 131 1.0% SULFUR, 0.1 NA, 0.1 V PPM

P, ATM	1.0000	1.0000	5.0000	5.0000	7.0000	7.0000	10.000	10.000
T, DEG K	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0
SOLUTION 1								
AR	8.8043-3	8.8048-3	8.8044-3	8.8052-3	8.8045-3	8.8052-3	8.8045-3	8.8053-3
CO	3.0470-9	9.383-12	1.3630-9	4.198-12	1.1520-9	3.548-12	9.638-10	2.969-12
CO2	9.0030-2	9.0036-2	9.0032-2	9.0039-2	9.0032-2	9.0040-2	9.0033-2	9.0041-2
H	5.830-12	4.799-15	1.744-12	1.435-15	1.355-12	1.115-15	1.037-12	8.536-16
HNO	1.514-12	1.651-14	2.265-12	2.468-14	2.463-12	2.684-14	2.693-12	2.935-14
HNO2	4.1475-9	1.6158-9	1.3866-8	5.4006-9	1.7845-8	6.9503-9	2.3317-8	9.0812-9
HNO3	1.222-11	1.528-11	9.133-11	1.142-10	1.391-10	1.739-10	2.172-10	2.715-10
HO2	1.2030-8	9.760-10	1.7980-8	1.4590-9	1.9560-8	1.5870-9	2.1380-8	1.7350-9
H2	2.5750-9	1.594-11	1.1520-9	7.132-12	9.736-10	6.028-12	8.146-10	5.044-12
H2O	9.6172-2	9.6178-2	9.6174-2	9.6182-2	9.6174-2	9.6182-2	9.6175-2	9.6182-2
H2O2	4.812-10	5.480-11	1.0760-9	1.225-10	1.2730-9	1.449-10	1.5220-9	1.732-10
H2SO4	2.7009-9	8.1478-8	2.7537-8	6.1724-7	4.4321-8	9.2328-7	7.3061-8	1.4041-6
NO	9.5128-5	1.4918-5	9.5117-5	1.4914-5	9.5114-5	1.4914-5	9.5110-5	1.4913-5
NO2	1.0155-6	5.2638-7	2.2702-6	1.1764-6	2.6859-6	1.3918-6	3.2100-6	1.6633-6
NO3	1.282-13	2.831-14	6.407-13	1.414-13	8.969-13	1.980-13	1.281-12	2.827-13
N2	7.3731-1	7.3739-1	7.3732-1	7.3742-1	7.3732-1	7.3743-1	7.3732-1	7.3743-1
N2O	5.6400-9	1.0162-9	1.2610-8	2.2719-9	1.4920-8	2.6880-9	1.7832-8	3.2126-9
NAOH	1.3280-9	1.139-12	6.598-10	2.509-12	3.859-10	1.344-13	3.987-10	1.663-12
NA2SO4	9.519-10	6.864-11	2.3970-9	2.5220-9	1.3200-9	1.083-11	2.3220-9	2.5210-9
O	3.5190-9	1.979-11	1.5730-9	8.850-12	1.3300-9	7.479-12	1.1120-9	6.257-12
OH	1.5463-6	5.5734-8	1.0340-6	3.7267-8	9.5058-7	3.4260-8	8.6947-7	3.1336-8
O2	6.7196-2	6.7181-2	6.7180-2	6.7144-2	6.7176-2	6.7136-2	6.7170-2	6.7128-2
O3	1.922-12	1.016-13	4.296-12	2.269-13	5.082-12	2.684-13	6.074-12	3.208-13
SO2	3.6407-4	2.4349-4	3.3204-4	1.6502-4	3.2262-4	1.4902-4	3.1148-4	1.3273-4
SO3	3.0810-5	1.5134-4	6.2824-5	2.2929-4	7.2224-5	2.4498-4	8.3340-5	2.6079-4
M, MOL WT	28.880	28.882	28.880	28.883	28.880	28.883	28.881	28.883
PHASE FRACTION	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0
SOLUTION 2								
NAOH(L)	1.0999-6	4.9968-8	0.000000	0.000000	2.2383-6	4.1273-8	0.000000	0.000000
NA2SO3(S)	0.000 0	5.550-12	0.000 0	0.000 0	0.000 0	2.317-12	0.000 0	0.000 0
NA2SO3(L)	5.150-11	0.000 0	0.000 0	0.000 0	1.890-10	0.000 0	0.000 0	0.000 0
NA2SO4(I)	0.000000	6.1231-1	0.000000	0.000000	0.000000	6.7620-1	0.000000	0.000000
NA2SO4(L)	1.4330-2	0.000000	0.000000	0.000000	1.3911-1	0.000000	0.000000	0.000000
NA2V2O6(L)	8.7555-1	2.2493-1	0.000000	0.000000	7.0996-1	3.8434-2	0.000000	0.000000
NA4V2O7(S)	9.2998-6	6.4247-8	0.000000	0.000000	0.000000	1.0699-9	0.000000	0.000000
V2O3(S)	3.3950-7	2.3950-9	0.000 0	0.000 0	6.6500-8	6.003-10	0.000 0	0.000 0
V2O5(L)	1.1011-1	1.6276-1	0.000000	0.000000	1.5093-1	2.8536-1	0.000000	0.000000
M, MOL WT	235.58	171.42	0.0000	0.0000	220.34	157.32	0.0000	0.0000
PHASE FRACTION	1.2484-9	3.1742-9	0.000000	0.000000	1.4294-9	3.8006-9	0.000000	0.000000
PURE SPECIES PHASE FRACTIONS (IF ANY)								
NA2V12O31(L)	0.000 0	0.000 0	0.000 0	2.051-10	0.000 0	0.000 0	2.051-10	2.051-10

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-11 FOR ALL ASSIGNED CONDITI

SOLUTION 1

C	CH	CH2	CH2O	CH2O2	CH3	CH2OH	CH3O	CH4	CH
CN	CN2	CNN	COS	CS	CS2	C2	C2H	C2H2	C2
C2H4	C2H4O2	C2H4O4	C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3	C2N	C2

C2O	C3	C3H6O	N-C3H7	I-C3H7	C3H8	1-C3H7OH	C3O2	C4	C4
N-C4H10	I-C4H10	C4N2	C5	C6H5	C6H5O	C6H6	C6H5OH	C7H8	C8
N-C8H18	I-C8H18	O-C12H9	C12H10	HCN	HCO	HNCO	H2N2	H2S	N
NCO	NH	NH2	NH3	N2H4	N2O4	N2O5	N3	NA	NA
NAH	NAO	NA2	NA2C2N2	NA2O	NA2O2H2	S	SH	SN	SO
S2	S2O	S8	V	VN	VO	VO2			

SOLUTION 2

NAOH(A)	NA2O(C)	NA2O(A)	NA2O(L)	NA2SO4(IV)	NA2V2O6(S)	NA6V2O8(S)	NA6V2O8(L)	V2O3(L)	V2

PURE SPECIES

C(GR)	C7H8(L)	C8H18(L)	H2O(S)	H2O(L)	H2SO4(L)	VN(S)	N2H6SO4(S)	NA(S)	NA
NACN(S)	NACN(L)	NAO2(S)	NA2CO3(1)	NA2CO3(2)	NA2CO3(L)	NA2O2(A)	NA2O2(B)	NA2S(1)	NA
NA2S(L)	S(S)	S(L)	V(S)	V(L)	NAVSO8(S)	NA2V12O31(S)	VO(S)	VO(L)	VO
VO2(S)	VO2(L)								

CASE NO. 8701 231 1.0% SULFUR, 1.0 NA, 0.1 V PPM TIME = 0.559 SEC

P, ATM	1.0000	1.0000	5.0000	5.0000	7.0000	7.0000	10.000	10.000	15.000	15.000
T, DEG K	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0
SOLUTION 1										
AR	8.8043-3	8.8048-3	8.8044-3	8.8052-3	8.8045-3	8.8052-3	8.8045-3	8.8053-3	8.8046-3	8.8054-3
CO	3.0470-9	9.383-12	1.3630-9	4.198-12	1.1520-9	3.548-12	9.638-10	2.969-12	7.870-10	2.424-12
CO2	9.0030-2	9.0035-2	9.0032-2	9.0039-2	9.0032-2	9.0040-2	9.0033-2	9.0041-2	9.0033-2	9.0041-2
H	5.830-12	4.799-15	1.744-12	1.435-15	1.355-12	1.115-15	1.037-12	8.536-16	7.650-13	6.298-16
HNO	1.514-12	1.651-14	2.265-12	2.468-14	2.463-12	2.684-14	2.693-12	2.935-14	2.980-12	3.248-14
HNO2	4.1475-9	1.6158-9	1.3866-8	5.4006-9	1.7845-8	6.9503-9	2.3317-8	9.0812-9	3.1601-8	1.2308-8
HNO3	1.222-11	1.528-11	9.133-11	1.142-10	1.391-10	1.739-10	2.172-10	2.715-10	3.605-10	4.506-10
HO2	1.2030-8	9.760-10	1.7980-8	1.4590-9	1.9560-8	1.5870-9	2.1380-8	1.7350-9	2.3660-8	1.9190-9
H2	2.5750-9	1.594-11	1.1520-9	7.132-12	9.736-10	6.028-12	8.146-10	5.044-12	6.651-10	4.119-12
H2O	9.6172-2	9.6178-2	9.6173-2	9.6181-2	9.6174-2	9.6182-2	9.6175-2	9.6182-2	9.6175-2	9.6182-2
H2O2	4.812-10	5.480-11	1.0760-9	1.225-10	1.2730-9	1.449-10	1.5220-9	1.732-10	1.8630-9	2.121-10
H2SO4	2.7008-9	8.1473-8	2.7536-8	6.1720-7	4.4318-8	9.2323-7	7.3056-8	1.4040-6	1.2811-7	2.2402-6
NO	9.5128-5	1.4918-5	9.5117-5	1.4914-5	9.5114-5	1.4914-5	9.5110-5	1.4913-5	9.5105-5	1.4912-5
NO2	1.0155-6	5.2638-7	2.2702-6	1.1764-6	2.6859-6	1.3918-6	3.2100-6	1.6633-6	3.9310-6	2.0369-6
NO3	1.282-13	2.831-14	6.407-13	1.414-13	8.969-13	1.980-13	1.281-12	2.827-13	1.921-12	4.240-13
N2	7.3731-1	7.3739-1	7.3732-1	7.3742-1	7.3732-1	7.3743-1	7.3732-1	7.3743-1	7.3733-1	7.3744-1
N2O	5.6400-9	1.0162-9	1.2610-8	2.2719-9	1.4920-8	2.6880-9	1.7832-8	3.2126-9	2.1839-8	3.9344-9
NAOH	6.4140-9	1.423-12	1.4850-9	2.314-13	9.987-10	1.599-13	6.540-10	1.085-13	4.045-10	7.012-14
NA2SO4	2.2220-8	1.071-10	1.2150-8	2.144-11	8.8390-9	1.532-11	6.2490-9	1.072-11	4.1910-9	7.150-12
O	3.5190-9	1.979-11	1.5730-9	8.850-12	1.3300-9	7.479-12	1.1120-9	6.257-12	9.083-10	5.109-12
OH	1.5463-6	5.5734-8	1.0340-6	3.7267-8	9.5058-7	3.4260-8	8.6947-7	3.1336-8	7.8564-7	2.8315-8
O2	6.7196-2	6.7181-2	6.7180-2	6.7144-2	6.7176-2	6.7136-2	6.7170-2	6.7128-2	6.7163-2	6.7120-2
O3	1.922-12	1.016-13	4.296-12	2.269-13	5.082-12	2.684-13	6.074-12	3.208-13	7.438-12	3.928-13
SO2	3.6405-4	2.4347-4	3.3202-4	1.6501-4	3.2260-4	1.4901-4	3.1146-4	1.3273-4	2.9732-4	1.1528-4
SO3	3.0808-5	1.5133-4	6.2820-5	2.2927-4	7.2220-5	2.4497-4	8.3335-5	2.6078-4	9.7424-5	2.7739-4
M, MOL WT	28.880	28.882	28.880	28.883	28.880	28.883	28.881	28.883	28.881	28.883
PHASE FRACTION	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0
SOLUTION 2										
NAOH(L)	5.3139-6	6.2416-8	6.1536-6	5.0737-8	5.7922-6	4.9089-8	5.4187-6	4.7580-8	5.0268-6	4.6135-8
NA2SO3(S)	0.000 0	8.659-12	0.000 0	3.878-12	0.000 0	3.278-12	0.000 0	2.743-12	0.000 0	2.240-12
NA2SO3(L)	1.2020-9	0.000 0	1.4700-9	0.000 0	1.2660-9	0.000 0	1.0690-9	0.000 0	8.785-10	0.000 0
NA2SO4(I)	0.000000	9.5333-1	0.000000	9.5637-1	0.000000	9.5650-1	0.000000	9.5659-1	0.000000	9.5667-1
NA2SO4(L)	3.3446-1	0.000000	9.1453-1	0.000000	9.3150-1	0.000000	9.4070-1	0.000000	9.4644-1	0.000000
NA2V2O6(L)	6.6180-1	3.0516-2	8.3774-2	9.6759-3	6.6383-2	6.9623-3	5.6375-2	4.8330-3	4.9122-2	3.1550-3
NA4V2O7(S)	1.6410-4	1.3600-8	5.5700-6	5.699-10	2.7930-6	2.742-10	1.4530-6	1.252-10	7.2650-7	5.121-11
NA6V2O8(S)	1.981-10	0.000 0	1.804-12	0.000 0	0.000 0	0.000 0	0.000 0	0.000 0	0.000 0	0.000 0
V2O3(S)	1.0990-8	2.082-10	1.0380-9	9.999-11	9.285-10	7.687-11	9.010-10	5.680-11	9.124-10	3.945-11
V2O5(L)	3.5659-3	1.4152-2	1.6831-3	3.3956-2	2.1074-3	3.6543-2	2.9213-3	3.8573-2	4.4367-3	4.0173-2
M, MOL WT	209.59	145.71	150.63	144.38	148.88	144.20	147.89	144.07	147.22	143.96
PHASE FRACTION	1.8489-9	2.7550-8	1.4398-8	2.8205-8	1.7966-8	2.8287-8	2.0752-8	2.8352-8	2.2975-8	2.8403-8

PURE SPECIES PHASE FRACTIONS (IF ANY)

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-11 FOR ALL ASSIGNED CONDITI

SOLUTION 1

C	CH	CH2	CH2O	CH2O2	CH3	CH2OH	CH3O	CH4	CH
CN	CN2	CNN	COS	CS	CS2	C2	C2H	C2H2	C2
C2H4	C2H4O2	C2H4O4	C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3	C2N	C2
C2O	C3	C3H6O	N-C3H7	I-C3H7	C3H8	1-C3H7OH	C3O2	C4	C4
N-C4H10	I-C4H10	C4N2	C5	C6H5	C6H5O	C6H6	C6H5OH	C7H8	C8
N-C8H18	I-C8H18	O-C12H9	C12H10	HCN	HCO	HNCO	H2N2	H2S	N
NCO	NH	NH2	NH3	N2H4	N2O4	N2O5	N3	NA	NA
NAH	NAO	NA2	NA2C2N2	NA2O	NA2O2H2	S	SH	SN	SO
S2	S2O	S8	V	VN	VO	VO2			

SOLUTION 2

NAOH(A)	NA2O(C)	NA2O(A)	NA2O(L)	NA2SO4(IV)	NA2V2O6(S)	NA6V2O8(L)	V2O3(L)	V2O5(S)

PURE SPECIES

C(GR)	C7H8(L)	C8H18(L)	H2O(S)	H2O(L)	H2SO4(L)	VN(S)	N2HBSO4(S)	NA(S)	NA
NACN(S)	NACN(L)	NAO2(S)	NA2CO3(1)	NA2CO3(2)	NA2CO3(L)	NA2O2(A)	NA2O2(B)	NA2S(1)	NA
NA2S(L)	S(S)	S(L)	V(S)	V(L)	NAV3O8(S)	NA2V12O31(S)	NA2V12O31(L)	VO(S)	VO
VO2(S)	VO2(S)	VO2(L)							

CASE NO. 8701 331 1.0% SULFUR, 10 NA, 0.1 V PPM TIME = 0.536 SEC

P, ATM	1.0000	1.0000	5.0000	5.0000	7.0000	7.0000	10.000	10.000	15.000	15.000
T, DEG K	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0
SOLUTION 1										
AR	8.8043-3	8.8048-3	8.8044-3	8.8052-3	8.8045-3	8.8052-3	8.8045-3	8.8053-3	8.8046-3	8.8054-3
CO	3.0470-9	9.383-12	1.3630-9	4.198-12	1.1520-9	3.548-12	9.638-10	2.969-12	7.870-10	2.424-12
CO2	9.0029-2	9.0035-2	9.0031-2	9.0038-2	9.0031-2	9.0039-2	9.0032-2	9.0040-2	9.0032-2	9.0041-2
H	5.830-12	4.799-15	1.744-12	1.435-15	1.355-12	1.115-15	1.037-12	8.536-16	7.650-13	6.298-16
HNO	1.514-12	1.651-14	2.265-12	2.468-14	2.463-12	2.684-14	2.693-12	2.935-14	2.980-12	3.248-14
HNO2	4.1475-9	1.6158-9	1.3866-8	5.4006-9	1.7845-8	6.9503-9	2.3317-8	9.0813-9	3.1602-8	1.2308-8
HNO3	1.222-11	1.528-11	9.133-11	1.142-10	1.391-10	1.739-10	2.172-10	2.715-10	3.605-10	4.506-10
HO2	1.2030-8	9.760-10	1.7980-8	1.4590-9	1.9560-8	1.5870-9	2.1380-8	1.7350-9	2.3660-8	1.9190-9
H2	2.5750-9	1.594-11	1.1520-9	7.132-12	9.736-10	6.028-12	8.146-10	5.044-12	6.651-10	4.118-12
H2O	9.6171-2	9.6177-2	9.6173-2	9.6181-2	9.6173-2	9.6181-2	9.6174-2	9.6182-2	9.6175-2	9.6182-2
H2O2	4.812-10	5.480-11	1.0760-9	1.225-10	1.2730-9	1.449-10	1.5220-9	1.732-10	1.8630-9	2.121-10
H2SO4	2.6991-9	8.1422-8	2.7519-8	6.1681-7	4.4291-8	9.2264-7	7.3010-8	1.4031-6	1.2803-7	2.2388-6
NO	9.5128-5	1.4918-5	9.5118-5	1.4915-5	9.5115-5	1.4914-5	9.5111-5	1.4913-5	9.5106-5	1.4912-5
NO2	1.0155-6	5.2639-7	2.2702-6	1.1764-6	2.6860-6	1.3918-6	3.2101-6	1.6633-6	3.9311-6	2.0369-6
NO3	1.282-13	2.831-14	6.407-13	1.414-13	8.969-13	1.980-13	1.281-12	2.827-13	1.921-12	4.240-13
N2	7.3731-1	7.3739-1	7.3732-1	7.3742-1	7.3732-1	7.3743-1	7.3733-1	7.3743-1	7.3733-1	7.3744-1
N2O	5.6401-9	1.0163-9	1.2610-8	2.2719-9	1.4920-8	2.6880-9	1.7832-8	3.2126-9	2.1839-8	3.9344-9
NA	1.431-12	4.644-18	6.000-14	2.257-19	3.106-14	1.212-19	1.549-14	6.292-20	7.047-15	3.001-20
NAOH	1.1060-8	1.453-12	1.5500-9	2.361-13	1.0330-9	1.632-13	6.730-10	1.107-13	4.150-10	7.155-14
NA2SO4	6.6020-8	1.116-10	1.3220-8	2.232-11	9.4450-9	1.594-11	6.6120-9	1.116-11	4.4080-9	7.440-12
O	3.5190-9	1.979-11	1.5730-9	8.850-12	1.3300-9	7.479-12	1.1120-9	6.257-12	9.083-10	5.109-12
OH	1.5463-6	5.5734-8	1.0340-6	3.7267-8	9.5058-7	3.4260-8	8.6947-7	3.1336-8	7.8564-7	2.8315-8
O2	6.7197-2	6.7182-2	6.7181-2	6.7145-2	6.7177-2	6.7137-2	6.7171-2	6.7130-2	6.7164-2	6.7121-2
O3	1.922-12	1.016-13	4.296-12	2.269-13	5.082-12	2.684-13	6.074-12	3.208-13	7.438-12	3.928-13
SO2	3.6382-4	2.4332-4	3.3181-4	1.6490-4	3.2240-4	1.4892-4	3.1127-4	1.3264-4	2.9713-4	1.1521-4
SO3	3.0789-5	1.5124-4	6.2781-5	2.2913-4	7.2175-5	2.4481-4	8.3283-5	2.6061-4	9.7363-5	2.7721-4
M, MOL WT	28.880	28.882	28.880	28.883	28.880	28.883	28.881	28.883	28.881	28.883
PHASE FRACTION	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0
SOLUTION 2										
NAOH(L)	9.1630-6	6.3734-8	6.4213-6	5.1781-8	5.9891-6	5.0095-8	5.5756-6	4.8553-8	5.1568-6	4.7077-8
NA2SO3(S)	0.000 0	9.023-12	0.000 0	4.036-12	0.000 0	3.411-12	0.000 0	2.854-12	0.000 0	2.331-12
NA2SO3(L)	3.5720-9	0.000 0	1.6000-9	0.000 0	1.3520-9	0.000 0	1.1310-9	0.000 0	9.239-10	0.000 0
NA2SO4(I)	0.000000	9.9549-1	0.000000	9.9550-1	0.000000	9.9550-1	0.000000	9.9551-1	0.000000	9.9551-1
NA2SO4(L)	9.9387-1	0.000000	9.9524-1	0.000000	9.9531-1	0.000000	9.9536-1	0.000000	9.9541-1	0.000000
NA2V2O6(L)	6.1029-3	3.1206-3	4.6702-3	1.0294-3	4.5482-3	7.4445-4	4.4138-3	5.1882-4	4.2262-3	3.3974-4
NA4V2O7(S)	4.4990-6	1.4500-9	3.3810-7	6.315-11	2.0460-7	3.053-11	1.2050-7	1.399-11	6.5780-8	5.742-12
NA6V2O8(S)	1.615-11	0.000 0	0.000 0	0.000 0	0.000 0	0.000 0	0.000 0	0.000 0	0.000 0	0.000 0
V2O3(S)	3.410-11	2.042-11	5.314-11	1.021-11	5.950-11	7.892-12	6.663-11	5.856-12	7.459-11	4.079-12
V2O5(L)	1.1059-5	1.3880-3	8.6165-5	3.4683-3	1.3505-4	3.7519-3	2.1602-4	3.9764-3	3.6271-4	4.1546-3
M, MOL WT	142.66	142.41	142.52	142.28	142.51	142.26	142.49	142.25	142.48	142.24
PHASE FRACTION	2.0111-7	2.7294-7	2.5869-7	2.7361-7	2.6274-7	2.7370-7	2.6577-7	2.7377-7	2.6815-7	2.7382-7

PURE SPECIES PHASE FRACTIONS (IF ANY)

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-11 FOR ALL ASSIGNED CONDITI

SOLUTION 1

C	CH	CH2	CH2O	CH2O2	CH3	CH2OH	CH3O	CH4	CH
CN	CN2	CNN	COS	CS	CS2	C2	C2H	C2H2	C2
C2H4	C2H4O2	C2H4O4	C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3	C2N	C2
C2O	C3	C3H6O	N-C3H7	I-C3H7	C3H8	1-C3H7OH	C3O2	C4	C4
N-C4H10	I-C4H10	C4N2	C5	C6H5	C6H5O	C6H6	C6H5OH	C7H8	C8
N-C8H18	I-C8H18	O-C12H9	C12H10	HCN	HCO	HNCO	H2N2	H2S	N
NCO	NH	NH2	NH3	N2H4	N2O4	N2O5	N3	NACN	NA
NAO	NA2	NA2C2N2	NA2O	NA2O2H2	S	SH	SN	SO	S2
S2O	S8	V	VN	VO	VO2				

SOLUTION 2

NAOH(A)	NA2O(C)	NA2O(A)	NA2O(L)	NA2SO4(IV)	NA2V2O6(S)	NA6V2O8(L)	V2O3(L)	V2O5(S)

PURE SPECIES

C(GR)	C7H8(L)	C8H18(L)	H2O(S)	H2O(L)	H2SO4(L)	VN(S)	N2H6SO4(S)	NA(S)	NA
NACN(S)	NACN(L)	NAO2(S)	NA2CO3(1)	NA2CO3(2)	NA2CO3(L)	NA2O2(A)	NA2O2(B)	NA2S(1)	NA
NA2S(L)	S(S)	S(L)	V(S)	V(L)	NAV3O8(S)	NA2V12O31(S)	NA2V12O31(L)	VO(S)	VO
VO2(S)	VO2(S)	VO2(L)							

CASE NO. 8701 132 1.0% SULFUR, 0.1 NA, 1.0 V PPM TIME = 0.681 SEC

P, ATM	1.0000	1.0000	5.0000	5.0000	7.0000	7.0000	10.000	10.000	15.000	15.000
T, DEG K	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0
SOLUTION 1										
AR	8.8043-3	8.8048-3	8.8044-3	8.8052-3	8.8045-3	8.8052-3	8.8045-3	8.8053-3	8.8046-3	8.8054-3
CO	3.0470-9	9.383-12	1.3630-9	4.198-12	1.1520-9	3.548-12	9.638-10	2.969-12	7.870-10	2.424-12
CO2	9.0030-2	9.0035-2	9.0032-2	9.0039-2	9.0032-2	9.0040-2	9.0033-2	9.0041-2	9.0033-2	9.0041-2
H	5.830-12	4.799-15	1.744-12	1.435-15	1.355-12	1.115-15	1.037-12	8.536-16	7.650-13	6.298-16
HNO	1.514-12	1.651-14	2.265-12	2.468-14	2.463-12	2.684-14	2.693-12	2.935-14	2.980-12	3.248-14
HNO2	4.1475-9	1.6158-9	1.3866-8	5.4006-9	1.7845-8	6.9503-9	2.3317-8	9.0812-9	3.1601-8	1.2308-8
HNO3	1.222-11	1.528-11	9.133-11	1.142-10	1.391-10	1.739-10	2.172-10	2.715-10	3.605-10	4.506-10
HO2	1.2030-8	9.760-10	1.7980-8	1.4590-9	1.9560-8	1.5870-9	2.1380-8	1.7350-9	2.3660-8	1.9190-9
H2	2.5750-9	1.594-11	1.1520-9	7.132-12	9.736-10	6.028-12	8.146-10	5.044-12	6.651-10	4.119-12
H2O	9.6172-2	9.6178-2	9.6173-2	9.6181-2	9.6174-2	9.6182-2	9.6175-2	9.6182-2	9.6175-2	9.6182-2
H2O2	4.812-10	5.480-11	1.0760-9	1.225-10	1.2730-9	1.449-10	1.5220-9	1.732-10	1.8630-9	2.121-10
H2SO4	2.7009-9	8.1478-8	2.7538-8	6.1724-7	4.4321-8	9.2328-7	7.3061-8	1.4041-6	1.2812-7	2.2403-6
NO	9.5128-5	1.4918-5	9.5117-5	1.4914-5	9.5114-5	1.4914-5	9.5110-5	1.4913-5	9.5105-5	1.4912-5
NO2	1.0155-6	5.2638-7	2.2702-6	1.1764-6	2.6859-6	1.3918-6	3.2100-6	1.6633-6	3.9310-6	2.0369-6
NO3	1.282-13	2.831-14	6.407-13	1.414-13	8.969-13	1.980-13	1.281-12	2.827-13	1.921-12	4.240-13
N2	7.3731-1	7.3739-1	7.3732-1	7.3742-1	7.3732-1	7.3743-1	7.3732-1	7.3743-1	7.3733-1	7.3744-1
N2O	5.6400-9	1.0162-9	1.2610-8	2.2719-9	1.4920-8	2.6880-9	1.7832-8	3.2126-9	2.1839-8	3.9344-9
NAOH	2.418-10	3.940-13	1.076-10	9.200-14	9.020-11	6.539-14	7.437-11	4.528-14	5.912-11	2.972-14
NA2SO4	3.158-11	8.212-12	6.380-11	3.391-12	7.210-11	2.563-12	8.079-11	1.869-12	8.953-11	1.285-12
O	3.5190-9	1.979-11	1.5730-9	8.850-12	1.3300-9	7.479-12	1.1120-9	6.257-12	9.083-10	5.109-12
OH	1.5463-6	5.5734-8	1.0340-6	3.7267-8	9.5058-7	3.4260-8	8.6947-7	3.1336-8	7.8564-7	2.8315-8
O2	6.7196-2	6.7181-2	6.7180-2	6.7144-2	6.7176-2	6.7136-2	6.7170-2	6.7128-2	6.7163-2	6.7120-2
O3	1.922-12	1.016-13	4.296-12	2.269-13	5.082-12	2.684-13	6.074-12	3.208-13	7.438-12	3.928-13
SO2	3.6407-4	2.4349-4	3.3204-4	1.6502-4	3.2263-4	1.4902-4	3.1148-4	1.3273-4	2.9734-4	1.1529-4
SO3	3.0810-5	1.5134-4	6.2824-5	2.2929-4	7.2224-5	2.4498-4	8.3340-5	2.6079-4	9.7431-5	2.7740-4
M, MOL WT	28.880	28.882	28.880	28.883	28.880	28.883	28.881	28.883	28.881	28.883
PHASE FRACTION	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0
SOLUTION 2										
NAOH(L)	2.0033-7	1.7283-8	4.4590-7	2.0176-8	5.2310-7	2.0077-8	6.1614-7	1.9862-8	7.3469-7	1.9535-8
NA2SO3(L)	1.708-12	0.000 0	7.719-12	0.000 0	1.032-11	0.000 0	1.383-11	0.000 0	1.877-11	0.000 0
NA2SO4(I)	0.000000	7.3253-2	0.000000	1.5124-1	0.000000	1.6001-1	0.000000	1.6671-1	0.000000	1.7189-1
NA2SO4(L)	4.7537-4	0.000000	4.8022-3	0.000000	7.5979-3	0.000000	1.2163-2	0.000000	2.0218-2	0.000000
NA2V206(L)	2.0862-1	1.3148-1	2.0620-1	3.6596-2	2.0285-1	2.5944-2	1.9725-1	1.7806-2	1.8740-1	1.1522-2
NA4V207(S)	7.3510-8	4.4930-9	7.1990-8	3.408-10	6.9620-8	1.709-10	6.5740-8	8.036-11	5.9210-8	3.360-11
V203(S)	2.4380-6	1.1700-8	4.8660-7	2.3920-9	3.4790-7	1.7120-9	2.4380-7	1.2010-9	1.6290-7	8.018-10
V205(L)	7.9091-1	7.9527-1	7.8899-1	8.1216-1	7.8955-1	8.1405-1	7.9058-1	8.1548-1	7.9238-1	8.1659-1
M, MOL WT	194.79	187.11	194.47	178.12	194.15	177.11	193.62	176.34	192.69	175.75
PHASE FRACTION	1.2311-8	1.3278-8	1.2365-8	1.4499-8	1.2399-8	1.4651-8	1.2457-8	1.4769-8	1.2559-8	1.4861-8

PURE SPECIES PHASE FRACTIONS (IF ANY)

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-11 FOR ALL ASSIGNED CONDITI

SOLUTION 1

C	CH	CH2	CH2O	CH2O2	CH3	CH2OH	CH3O	CH4	CH
CN	CN2	CNN	COS	CS	CS2	C2	C2H	C2H2	C2
C2H4	C2H4O2	C2H4O4	C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3	C2N	C2
C2O	C3	C3H6O	N-C3H7	I-C3H7	C3H8	1-C3H7OH	C3O2	C4	C4
N-C4H10	I-C4H10	C4N2	C5	C6H5	C6H5O	C6H6	C6H5OH	C7H8	C8
N-C8H18	I-C8H18	O-C12H9	C12H10	HCN	HCO	HNCO	H2N2	H2S	N
NCO	NH	NH2	NH3	N2H4	N2O4	N2O5	N3	NA	NA
NAH	NAO	NA2	NA2C2N2	NA2O	NA2O2H2	S	SH	SN	SO
S2	S2O	S8	V	VN	VO	VO2			

SOLUTION 2

NAOH(A)	NA2O(C)	NA2O(A)	NA2O(L)	NA2SO3(S)	NA2SO4(IV)	NA2V2O6(S)	NA6V2O8(S)	NA6V2O8(L)	V2
V2O5(S)									

PURE SPECIES

C(GR)	C7H8(L)	C8H18(L)	H2O(S)	H2O(L)	H2SO4(L)	VN(S)	N2H6SO4(S)	NA(S)	NA
NACN(S)	NACN(L)	NAO2(S)	NA2CO3(1)	NA2CO3(2)	NA2CO3(L)	NA2O2(A)	NA2O2(B)	NA2S(1)	NA
NA2S(L)	S(S)	S(L)	V(S)	V(L)	NAV3O8(S)	NA2V12O31(S)	NA2V12O31(L)	VO(S)	VO
VO2(S)	VO2(S)	VO2(L)							

CASE NO. 8701 232 1.0% SULFUR, 1.0 NA, 1.0 V PPM TIME = 0.733 SEC

P, ATM	1.0000	1.0000	5.0000	5.0000	7.0000	7.0000	10.000	10.000	15.000	15.000
T, DEG K	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0
SOLUTION 1										
AR	8.8043-3	8.8048-3	8.8044-3	8.8052-3	8.8045-3	8.8052-3	8.8045-3	8.8053-3	8.8046-3	8.8054-3
CO	3.0470-9	9.383-12	1.3630-9	4.198-12	1.1520-9	3.548-12	9.638-10	2.969-12	7.870-10	2.424-12
CO2	9.0030-2	9.0035-2	9.0031-2	9.0039-2	9.0032-2	9.0040-2	9.0032-2	9.0041-2	9.0033-2	9.0041-2
H	5.830-12	4.799-15	1.744-12	1.435-15	1.355-12	1.115-15	1.037-12	8.536-16	7.650-13	6.298-16
HNO	1.514-12	1.651-14	2.265-12	2.468-14	2.463-12	2.684-14	2.693-12	2.935-14	2.980-12	3.248-14
HNO2	4.1475-9	1.6158-9	1.3866-8	5.4006-9	1.7845-8	6.9503-9	2.3317-8	9.0812-9	3.1601-8	1.2308-8
HNO3	1.222-11	1.528-11	9.133-11	1.142-10	1.391-10	1.739-10	2.172-10	2.715-10	3.605-10	4.506-10
HO2	1.2030-8	9.760-10	1.7980-8	1.4590-9	1.9560-8	1.5870-9	2.1380-8	1.7350-9	2.3660-8	1.9190-9
H2	2.5750-9	1.594-11	1.1520-9	7.132-12	9.736-10	6.028-12	8.146-10	5.044-12	6.651-10	4.119-12
H2O	9.6172-2	9.6178-2	9.6173-2	9.6181-2	9.6174-2	9.6182-2	9.6174-2	9.6182-2	9.6175-2	9.6182-2
H2O2	4.812-10	5.490-11	1.0760-9	1.225-10	1.2730-9	1.449-10	1.5220-9	1.732-10	1.8630-9	2.121-10
H2SO4	2.7008-9	8.1474-8	2.7537-8	6.1720-7	4.4320-8	9.2323-7	7.3058-8	1.4040-6	1.2812-7	2.2402-6
NO	9.5128-5	1.4918-5	9.5117-5	1.4914-5	9.5114-5	1.4914-5	9.5110-5	1.4913-5	9.5105-5	1.4912-5
NO2	1.0155-6	5.2638-7	2.2702-6	1.1764-6	2.6859-6	1.3918-6	3.2100-6	1.6633-6	3.9310-6	2.0369-6
NO3	1.282-13	2.831-14	6.407-13	1.414-13	8.969-13	1.980-13	1.281-12	2.827-13	1.921-12	4.240-13
N2	7.3731-1	7.3739-1	7.3732-1	7.3742-1	7.3732-1	7.3743-1	7.3732-1	7.3743-1	7.3733-1	7.3744-1
N2O	5.6400-9	1.0162-9	1.2610-8	2.2719-9	1.4920-8	2.6880-9	1.7832-8	3.2126-9	2.1839-8	3.9344-9
NAOH	4.4220-9	1.146-12	1.0180-9	1.939-13	7.089-10	1.345-13	4.784-10	9.152-14	3.040-10	5.928-14
NA2SO4	1.0560-8	6.943-11	5.7020-9	1.506-11	4.4530-9	1.084-11	3.3430-9	7.633-12	2.3680-9	5.110-12
O	3.5190-9	1.979-11	1.5730-9	8.850-12	1.3300-9	7.479-12	1.1120-9	6.257-12	9.083-10	5.109-12
OH	1.5463-6	5.5734-8	1.0340-6	3.7267-8	9.5058-7	3.4260-8	8.6947-7	3.1336-8	7.8564-7	2.8315-8
O2	6.7197-2	6.7181-2	6.7180-2	6.7144-2	6.7176-2	6.7136-2	6.7170-2	6.7129-2	6.7163-2	6.7120-2
O3	1.922-12	1.016-13	4.296-12	2.269-13	5.082-12	2.684-13	6.074-12	3.208-13	7.438-12	3.928-13
SO2	3.6406-4	2.4347-4	3.3203-4	1.6501-4	3.2261-4	1.4901-4	3.1147-4	1.3273-4	2.9733-4	1.1528-4
SO3	3.0809-5	1.5133-4	6.2822-5	2.2927-4	7.2222-5	2.4497-4	8.3337-5	2.6078-4	9.7426-5	2.7739-4
M, MOL WT	28.880	28.882	28.880	28.883	28.880	28.883	28.881	28.883	28.881	28.883
PHASE FRACTION	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0
SOLUTION 2										
NAOH(L)	3.6636-6	5.0256-8	4.2158-6	4.2527-8	4.1113-6	4.1299-8	3.9632-6	4.0141-8	3.7781-6	3.9004-8
NA2SO3(S)	0.000 0	5.614-12	0.000 0	2.724-12	0.000 0	2.320-12	0.000 0	1.952-12	0.000 0	1.601-12
NA2SO3(L)	5.714-10	0.000 0	6.900-10	0.000 0	6.376-10	0.000 0	5.720-10	0.000 0	4.962-10	0.000 0
NA2SO4(I)	0.000000	6.1936-1	0.000000	6.7190-1	0.000000	6.7702-1	0.000000	6.8085-1	0.000000	6.8377-1
NA2SO4(L)	1.5898-1	0.000000	4.2925-1	0.000000	4.6932-1	0.000000	5.0324-1	0.000000	5.3465-1	0.000000
NA2V2O6(L)	8.3149-1	2.2190-1	5.4731-1	5.4729-2	4.9921-1	3.8380-2	4.5288-1	2.6131-2	4.0120-1	1.6807-2
NA4V2O7(S)	9.7990-5	6.4120-8	1.7080-5	2.2650-9	1.0580-5	1.0700-9	6.2450-6	4.817-10	3.3520-6	1.950-10
NA6V2O8(S)	5.624-11	0.000 0	2.596-12	0.000 0	1.093-12	0.000 0	0.000 0	0.000 0	0.000 0	0.000 0
V2O3(S)	2.9060-8	2.3360-9	1.4450-8	8.050-10	1.3860-8	5.987-10	1.3530-8	4.315-10	1.3190-8	2.940-10
V2O5(L)	9.4255-3	1.5874-1	2.3427-2	2.7338-1	3.1456-2	2.8460-1	4.3870-2	2.9302-1	6.4147-2	2.9942-1
M, MOL WT	227.09	170.96	198.70	158.50	194.12	157.28	189.90	156.37	185.44	155.68
PHASE FRACTION	1.4631-8	3.2329-8	2.1560-8	3.7507-8	2.3188-8	3.8102-8	2.4771-8	3.8560-8	2.6443-8	3.8917-8

PURE SPECIES PHASE FRACTIONS (IF ANY)

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-11 FOR ALL ASSIGNED CONDITI

SOLUTION 1

C	CH	CH2	CH2O	CH2O2	CH3	CH2OH	CH3O	CH4	CH
CN	CN2	CNN	COS	CS	CS2	C2	C2H	C2H2	C2
C2H4	C2H4O2	C2H4O4	C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3	C2N	C2
C2O	C3	C3H6O	N-C3H7	I-C3H7	C3H8	1-C3H7OH	C3O2	C4	C4
N-C4H10	I-C4H10	C4N2	C5	C6H5	C6H5O	C6H6	C6H5OH	C7H8	C8
N-C8H18	I-C8H18	O-C12H9	C12H10	HCN	HCO	HNCO	H2N2	H2S	N
NCO	NH	NH2	NH3	N2H4	N2O4	N2O5	N3	NA	NA
NAH	NAO	NA2	NA2CO2	NA2O	NA2O2H2	S	SH	SN	SO
S2	S2O	S8	V	VN	VO	VO2			

SOLUTION 2

NAOH(A)	NA2O(C)	NA2O(A)	NA2O(L)	NA2SO4(IV)	NA2V2O6(S)	NA6V2O8(L)	V2O3(L)	V2O5(S)

PURE SPECIES

C(GR)	C7H8(L)	C8H18(L)	H2O(S)	H2O(L)	H2SO4(L)	VN(S)	N2H6SO4(S)	NA(S)	NA
NACN(S)	NACN(L)	NAO2(S)	NA2CO3(1)	NA2CO3(2)	NA2CO3(L)	NA2O2(A)	NA2O2(B)	NA2S(1)	NA
NA2S(L)	S(S)	S(L)	V(S)	V(L)	NAV3O8(S)	NA2V12O31(S)	NA2V12O31(L)	VO(S)	VO
VO2(S)	VO2(S)	VO2(L)							

CASE NO. 8701 332 1.0% SULFUR, 10 NA, 1.0 V PPM singular matrix, iteration 29 variable 7

P, ATM	1.0000	1.0000
T, DEG K	1172.0	977.0
SOLUTION 1		
AR	8.8043-3	8.8048-3
CO	3.0470-9	9.383-12
CO2	9.0029-2	9.0035-2
H	5.830-12	4.799-15
HNO	1.514-12	1.651-14
HNO2	4.1475-9	1.6158-9
HNO3	1.222-11	1.528-11
HO2	1.2030-8	9.760-10
H2	2.5750-9	1.594-11
H2O	9.6171-2	9.6177-2
H2O2	4.812-10	5.480-11
H2SO4	2.6992-9	8.1423-8
NO	9.5129-5	1.4918-5
NO2	1.0155-6	5.2639-7
N2	7.3731-1	7.3739-1
N2O	5.6401-9	1.0163-9
NA	1.392-12	4.550-18
NAOH	1.0760-8	1.424-12
NA2SO4	6.2430-8	1.071-10
O	3.5190-9	1.979-11
OH	1.5463-6	5.5734-8
O2	6.7198-2	6.7182-2
O3	1.922-12	1.016-13
SO2	3.6383-4	2.4332-4
SO3	3.0790-5	1.5124-4
M, MOL WT	28.880	28.882
PHASE FRACTION	1.0000 0	1.0000 0
SOLUTION 2		
NAOH(L)	8.9107-6	6.2440-8
NA2SO3(S)	0.000 0	8.660-12
NA2SO3(L)	3.3780-9	0.000000
NA2SO4(I)	0.000000	9.5549-1
NA2SO4(L)	9.3993-1	0.000000
NA2V2O6(L)	5.9908-2	3.0416-2
NA4V2O7(S)	4.1765-5	1.3566-8
NA6V2O8(S)	1.418-10	0.000 0
V2O3(S)	3.539-10	2.074-10
V2O5(L)	1.1479-4	1.4095-2
M, MOL WT	148.15	145.70
PHASE FRACTION	2.0486-7	2.7646-7

PURE SPECIES PHASE FRACTIONS (IF ANY)

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-11 FOR ALL ASSIGNED CONDITI

SOLUTION 1

C	CH	CH2	CH2O	CH2O2	CH3	CH2OH	CH3O	CH4	CH
CN	CN2	CNN	COS	CS	CS2	C2	C2H	C2H2	C2
C2H4	C2H4O2	C2H4O4	C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3	C2N	C2
C2O	C3	C3H6O	N-C3H7	I-C3H7	C3H8	1-C3H7OH	C3O2	C4	C4
N-C4H10	I-C4H10	C4N2	C5	C6H5	C6H5O	C6H6	C6H5OH	C7H8	C8
N-C8H18	I-C8H18	O-C12H9	C12H10	HCN	HCO	HNCO	H2N2	H2S	N
NCO	NH	NH2	NH3	NO3	N2H4	N2O4	N2O5	NS	NA
NAH	NAO	NA2	NA2C2N2	NA2O	NA2O2H2	S	SH	SN	SO
S2	S2O	S8	V	VN	VO	VO2			

SOLUTION 2

NAOH(A)	NA2O(C)	NA2O(A)	NA2O(L)	NA2SO4(IV)	NA2V2O6(S)	NA6V2O8(L)	V2O3(L)	V2O5(S)

PURE SPECIES

C(GR)	C7H8(L)	C8H18(L)	H2O(S)	H2O(L)	H2SO4(L)	VN(S)	N2H6SO4(S)	NA(S)	NA
NACN(S)	NACN(L)	NAO2(S)	NA2CO3(1)	NA2CO3(2)	NA2CO3(L)	NA2O2(A)	NA2O2(B)	NA2S(1)	NA
NA2S(L)	S(S)	S(L)	V(S)	V(L)	NAV3O8(S)	NA2V12O31(S)	NA2V12O31(L)	VO(S)	VO
VO2(S)	VO2(S)	VO2(L)							

CASE NO. 8701 133 1.0% SULFUR, 0.1 NA, 10 V PPM TIME = 0.571 SEC

P, ATM	1.0000	1.0000	5.0000	5.0000	7.0000	7.0000	10.000	10.000	15.000	15.000
T, DEG K	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0
SOLUTION 1										
AR	8.8043-3	8.8048-3	8.8044-3	8.8052-3	8.8045-3	8.8052-3	8.8045-3	8.8053-3	8.8046-3	8.8054-3
CO	3.0470-9	9.3833-12	1.3630-9	4.198-12	1.1520-9	3.548-12	9.638-10	2.969-12	7.870-10	2.424-12
CO2	9.0029-2	9.0035-2	9.0031-2	9.0038-2	9.0031-2	9.0039-2	9.0032-2	9.0040-2	9.0032-2	9.0041-2
H	5.830-12	4.799-15	1.744-12	1.435-15	1.355-12	1.115-15	1.037-12	8.536-16	7.650-13	6.298-16
HNO	1.514-12	1.651-14	2.265-12	2.468-14	2.463-12	2.684-14	2.693-12	2.935-14	2.990-12	3.249-14
HNO2	4.1475-9	1.6158-9	1.3866-8	5.4006-9	1.7845-8	6.9503-9	2.3317-8	9.0813-9	3.1602-8	1.2308-8
HNO3	1.222-11	1.529-11	9.133-11	1.142-10	1.391-10	1.739-10	2.172-10	2.715-10	3.605-10	4.506-10
HO2	1.2030-8	9.760-10	1.7990-8	1.4590-9	1.9560-8	1.5870-9	2.1380-8	1.7350-9	2.3660-8	1.9190-9
H2	2.5750-9	1.594-11	1.1520-9	7.132-12	9.736-10	6.028-12	8.146-10	5.044-12	6.651-10	4.118-12
H2O	9.6171-2	9.6177-2	9.6173-2	9.6181-2	9.6173-2	9.6181-2	9.6174-2	9.6182-2	9.6175-2	9.6182-2
H2O2	4.812-10	5.490-11	1.0760-9	1.225-10	1.2730-9	1.449-10	1.5220-9	1.732-10	1.8630-9	2.121-10
H2SO4	2.7009-9	8.1477-8	2.7537-8	6.1723-7	4.4321-8	9.2327-7	7.3060-8	1.4041-6	1.2812-7	2.2403-6
NO	9.5128-5	1.4918-5	9.5118-5	1.4915-5	9.5115-5	1.4914-5	9.5111-5	1.4913-5	9.5106-5	1.4912-5
NO2	1.0155-6	5.2639-7	2.2702-6	1.1764-6	2.6860-6	1.3918-6	3.2101-6	1.6633-6	3.9311-6	2.0369-6
NO3	1.282-13	2.831-14	6.407-13	1.414-13	8.969-13	1.980-13	1.281-12	2.827-13	1.921-12	4.240-13
N2	7.3731-1	7.3739-1	7.3732-1	7.3742-1	7.3732-1	7.3743-1	7.3733-1	7.3743-1	7.3733-1	7.3744-1
N2O	5.6401-9	1.0163-9	1.2610-8	2.2719-9	1.4920-8	2.6880-9	1.7832-8	3.2126-9	2.1839-8	3.9344-9
NAOH	7.030-11	1.206-13	3.127-11	3.072-14	2.629-11	2.206-14	2.179-11	1.539-14	1.748-11	1.016-14
NA2SO4	2.669-12	7.692-13	5.384-12	3.782-13	6.124-12	2.916-13	6.935-12	2.160-13	7.826-12	1.502-13
O	3.5190-9	1.979-11	1.5730-9	8.850-12	1.3300-9	7.479-12	1.1120-9	6.257-12	9.083-10	5.109-12
OH	1.5463-6	5.5734-8	1.0340-6	3.7267-8	9.5058-7	3.4260-8	8.6947-7	3.1336-8	7.8564-7	2.8315-8
O2	6.7197-2	6.7182-2	6.7181-2	6.7145-2	6.7177-2	6.7137-2	6.7171-2	6.7129-2	6.7164-2	6.7121-2
O3	1.922-12	1.016-13	4.296-12	2.269-13	5.082-12	2.684-13	6.074-12	3.208-13	7.438-12	3.928-13
SO2	3.6407-4	2.4348-4	3.3204-4	1.6502-4	3.2262-4	1.4902-4	3.1148-4	1.3273-4	2.9734-4	1.1529-4
SO3	3.0810-5	1.5134-4	6.2824-5	2.2929-4	7.2224-5	2.4498-4	8.3340-5	2.6079-4	9.7430-5	2.7740-4
M, MOL WT	28.880	28.882	28.880	28.883	28.880	28.883	28.881	28.883	28.881	28.883
PHASE FRACTION	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0
SOLUTION 2										
NAOH(L)	5.8244-8	5.2894-9	1.2954-7	6.7381-9	1.5245-7	6.7725-9	1.8052-7	6.7517-9	2.1721-7	6.6869-9
NA2SO3(L)	0.000 0	0.000 0	0.000 0	0.000 0	0.000 0	0.000 0	1.187-12	0.000 0	1.640-12	0.000 0
NA2SO4(I)	0.000000	6.8613-3	0.000000	1.6868-2	0.000000	1.8207-2	0.000000	1.9263-2	0.000000	2.0099-2
NA2SO4(L)	4.0184-5	0.000000	4.0530-4	0.000000	6.4534-4	0.000000	1.0441-3	0.000000	1.7672-3	0.000000
NA2V2O6(L)	2.1810-2	1.5145-2	2.1573-2	4.9163-3	2.1342-2	3.5476-3	2.0946-2	2.4682-3	2.0217-2	1.6140-3
NA4V2O7(S)	6.496-10	4.847-11	6.357-10	5.107-12	6.221-10	2.659-12	5.993-10	1.287-12	5.583-10	0.000 0
V2O3(S)	3.0160-6	1.4390-8	6.0320-7	2.8800-9	4.3090-7	2.0580-9	3.0160-7	1.4410-9	2.0110-7	9.606-10
V2O5(L)	9.7815-1	9.7799-1	9.7802-1	9.7822-1	9.7801-1	9.7825-1	9.7801-1	9.7827-1	9.7802-1	9.7829-1
M, MOL WT	183.23	182.55	183.20	181.51	183.18	181.37	183.14	181.27	183.06	181.18
PHASE FRACTION	1.2305-7	1.2391-7	1.2310-7	1.2517-7	1.2313-7	1.2534-7	1.2318-7	1.2548-7	1.2327-7	1.2559-7

PURE SPECIES PHASE FRACTIONS (IF ANY)

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-11 FOR ALL ASSIGNED CONDITI

SOLUTION 1

C	CH	CH2	CH2O	CH2O2	CH3	CH2OH	CH3O	CH4	CH
CN	CN2	CNN	COS	CS	CS2	C2	C2H	C2H2	C2
C2H4	C2H4O2	C2H4O4	C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3	C2N	C2
C2O	C3	C3H6O	N-C3H7	I-C3H7	C3H8	1-C3H7OH	C3O2	C4	C4
N-C4H10	I-C4H10	C4N2	C5	C6H5	C6H5O	C6H6	C6H5OH	C7H8	C8
N-C8H18	I-C8H18	O-C12H9	C12H10	HCN	HCO	HNCO	H2N2	H2S	N
NCO	NH	NH2	NH3	N2H4	N2O4	N2O5	N3	NA	NA
NAH	NAO	NA2	NA2CO2	NA2O	NA2O2H2	S	SH	SN	SO
SO2	SO3	S8	V	VN	VO	VO2			

SOLUTION 2

NAOH(A)	NA2O(C)	NA2O(A)	NA2O(L)	NA2SO3(S)	NA2SO4(IV)	NA2V2O6(S)	NA6V2O8(S)	NA6V2O8(L)	V2
V2O5(S)									

PURE SPECIES

C(GR)	C7H8(L)	C8H18(L)	H2O(S)	H2O(L)	H2SO4(L)	VN(S)	N2H6SO4(S)	NA(S)	NA
NAOH(S)	NAOH(L)	NAO2(S)	NA2CO3(I)	NA2CO3(2)	NA2CO3(L)	NA2O2(A)	NA2O2(B)	NA2S(1)	NA
NA2S(L)	S(S)	S(L)	V(S)	V(L)	NAV3O8(S)	NA2V12O31(S)	NA2V12O31(L)	VO(S)	VO
VO2(S)	VO2(S)	VO2(L)							

CASE NO. 8701 233 1.0% SULFUR, 1.0 NA, 10 V PPM TIME = 0.728 SEC

P, ATM	1.0000	1.0000	5.0000	5.0000	7.0000	7.0000	10.000	10.000	15.000	15.000
T, DEG K	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0	1172.0	977.0
SOLUTION 1										
AR	8.8043-3	8.8048-3	8.8044-3	8.8052-3	8.8045-3	8.8052-3	8.8045-3	8.8053-3	8.8046-3	8.8054-3
CO	3.0470-9	9.3831-12	1.3630-9	4.1981-12	1.1520-9	3.5481-12	9.6381-10	2.9691-12	7.8701-10	2.4241-12
CO2	9.0029-2	9.0035-2	9.0031-2	9.0038-2	9.0031-2	9.0039-2	9.0032-2	9.0040-2	9.0032-2	9.0041-2
H	5.8301-12	4.7991-15	1.7441-12	1.4351-15	1.3551-12	1.1151-15	1.0371-12	8.5361-16	7.6501-13	6.2991-16
HNO	1.5141-12	1.6511-14	2.2651-12	2.4681-14	2.4631-12	2.6841-14	2.6931-12	2.9351-14	2.9801-12	3.2481-14
HNO2	4.1475-9	1.6158-9	1.3866-8	5.4006-9	1.7845-8	6.9503-9	2.3317-8	9.0813-9	3.1602-8	1.2308-8
HNO3	1.2221-11	1.5281-11	9.1331-11	1.1421-10	1.3911-10	1.7391-10	2.1721-10	2.7151-10	3.3051-10	4.5061-10
HO2	1.2030-8	9.7601-10	1.7981-8	1.4591-9	1.9561-8	1.5871-9	2.1381-8	1.7351-9	2.3661-8	1.9191-9
H2	2.5751-9	1.5941-11	1.1521-9	7.1321-12	9.7361-10	6.0281-12	8.1461-10	5.0441-12	6.6511-10	4.1181-12
H2O	9.6171-2	9.6171-2	9.6171-2	9.6181-2	9.6171-2	9.6181-2	9.6171-2	9.6181-2	9.6171-2	9.6181-2
H2O2	4.8121-10	5.4801-11	1.0761-9	1.2251-10	1.2731-9	1.4491-10	1.5221-9	1.7321-10	1.8631-9	2.1211-10
H2SO4	2.7001-9	8.1471-8	2.7531-8	6.1721-7	4.4321-8	9.2321-7	7.3061-8	1.4041-6	1.2811-7	2.2401-6
NO	9.5121-5	1.4911-5	9.5111-5	1.4911-5	9.5111-5	1.4911-5	9.5111-5	1.4911-5	9.5101-5	1.4911-5
NO2	1.0151-6	5.2631-7	2.2701-6	1.1761-6	2.6861-6	1.3911-6	3.2101-6	1.6631-6	3.9311-6	2.0361-6
NO3	1.2821-13	2.8311-14	6.4071-13	1.4141-13	8.9691-13	1.9801-13	1.2811-12	2.8271-13	1.9211-12	4.2401-13
N2	7.3731-1	7.3731-1	7.3731-1	7.3741-1	7.3731-1	7.3741-1	7.3731-1	7.3741-1	7.3731-1	7.3741-1
N2O	5.6401-9	1.0161-9	1.2611-8	2.2711-9	1.4921-8	2.6881-9	1.7831-8	3.2121-9	2.1831-8	3.9341-9
NAOH	2.4991-10	3.9461-13	1.1041-10	9.2051-14	9.2451-11	6.5421-14	7.6221-11	4.5301-14	6.0571-11	2.9731-14
NA2SO4	3.3721-11	8.2361-12	6.7061-11	3.3941-12	7.5741-11	2.5641-12	8.4861-11	1.8701-12	9.3981-11	1.2851-12
O	3.5191-9	1.9791-11	1.5731-9	8.8501-12	1.3301-9	7.4791-12	1.1121-9	6.2571-12	9.0831-10	5.1091-12
OH	1.5461-6	5.5731-8	1.0341-6	3.7261-8	9.5051-7	3.4261-8	8.6941-7	3.1331-8	7.8561-7	2.8311-8
O2	6.7191-2	6.7181-2	6.7181-2	6.7141-2	6.7171-2	6.7131-2	6.7171-2	6.7131-2	6.7161-2	6.7121-2
O3	1.9221-12	1.0161-13	4.2961-12	2.2691-13	5.0831-12	2.6841-13	6.0741-12	3.2081-13	7.4381-12	3.9281-13
SO2	3.6401-4	2.4341-4	3.3201-4	1.6501-4	3.2261-4	1.4901-4	3.1141-4	1.3271-4	2.9731-4	1.1521-4
SO3	3.0811-5	1.5131-4	6.2821-5	2.2921-4	7.2221-5	2.4491-4	8.3331-5	2.6071-4	9.7431-5	2.7731-4
M, MOL WT	28.880	28.882	28.880	28.883	28.880	28.883	28.881	28.883	28.881	28.883
PHASE FRACTION	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0	1.0000 0
SOLUTION 2										
NAOH(L)	2.0701-7	1.7301-8	4.5711-7	2.0181-8	5.3611-7	2.0081-8	6.3141-7	1.9861-8	7.5271-7	1.9531-8
NA2SO3(L)	1.8251-12	0.000 0	8.1141-12	0.000 0	1.0841-11	0.000 0	1.4521-11	0.000 0	1.9701-11	0.000 0
NA2SO4(I)	0.000000	7.3461-2	0.000000	1.5131-1	0.000000	1.6011-1	0.000000	1.6681-1	0.000000	1.7191-1
NA2SO4(L)	5.0761-4	0.000000	5.0471-3	0.000000	7.9821-3	0.000000	1.2771-2	0.000000	2.1221-2	0.000000
NA2V2O6(L)	2.1961-1	1.3171-1	2.1431-1	3.6621-2	2.1081-1	2.5761-2	2.0491-1	1.7811-2	1.9461-1	1.1521-2
NA4V2O7(S)	8.2661-8	4.5161-9	7.8691-8	3.4151-10	7.6021-8	1.7111-10	7.1761-8	8.0441-11	6.4561-8	3.3631-11
V2O3(S)	2.4041-6	1.1691-8	4.8141-7	2.3911-9	3.4421-7	1.7121-9	2.4131-7	1.2011-9	1.6121-7	8.0171-10
V2O5(L)	7.7981-1	7.9471-1	7.8051-1	8.1191-1	7.8111-1	8.1391-1	7.8221-1	8.1531-1	7.8411-1	8.1631-1
M, MOL WT	195.47	187.12	194.97	178.12	194.63	177.11	194.08	176.34	193.10	175.74
PHASE FRACTION	1.2311-7	1.3281-7	1.2361-7	1.4501-7	1.2401-7	1.4651-7	1.2461-7	1.4771-7	1.2571-7	1.4861-7

PURE SPECIES PHASE FRACTIONS (IF ANY)

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-11 FOR ALL ASSIGNED CONDITI

SOLUTION 1

C	CH	CH2	CH2O	CH2O2	CH3	CH2OH	CH3O	CH4	CH
CN	CN2	CNN	COS	CS	CS2	C2	C2H	C2H2	C2
C2H4	C2H4O2	C2H4O4	C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3	C2N	C2
C2O	C3	C3H6O	N-C3H7	I-C3H7	C3H8	I-C3H7OH	C3O2	C4	C4
N-C4H10	I-C4H10	C4N2	C5	C5H5	C5H5O	C6H6	C6H5OH	C7H8	C8
N-C8H18	I-C8H18	O-C12H9	C12H10	HCN	HCO	HNCO	H2N2	H2S	N
NCO	NH	NH2	NH3	N2H4	N2O4	N2O5	N3	NA	NA
NAH	NAO	NA2	NA2C2N2	NA2O	NA2O2H2	S	SH	SN	SO
S2	S2O	S8	V	VN	VO	VO2			

SOLUTION 2

NAOH(A)	NA2O(C)	NA2O(A)	NA2O(L)	NA2SO3(S)	NA2SO4(IV)	NA2V2O6(S)	NA6V2O8(S)	NA6V2O8(L)	V2
V2O5(S)									

PURE SPECIES

C(GR)	C7H8(L)	C8H18(L)	H2O(S)	H2O(L)	H2SO4(L)	VN(S)	N2H6SO4(S)	NA(S)	NA
NACN(S)	NACN(L)	NAO2(S)	NA2CO3(1)	NA2CO3(2)	NA2CO3(L)	NA2O2(A)	NA2O2(B)	NA2S(1)	NA
NA2S(L)	S(S)	S(L)	V(S)	V(L)	NAV3O8(S)	NA2V12O31(S)	NA2V12O31(L)	VO(S)	VO
VO2(S)	VO2(S)	VO2(L)							

CASE NO. 8701 333 1.0% SULFUR, 10 NA, 10 V PPM singular matrix, iteration 27 variable 1

P, ATM	1.0000	1.0000
T, DEG K	1172.0	977.0
SOLUTION 1		
AR	8.8043-3	8.8048-3
CO	3.0470-9	9.383-12
CO2	9.0028-2	9.0034-2
H	5.830-12	4.799-15
HNO	1.514-12	1.651-14
HNO2	4.1476-9	1.6158-9
HNO3	1.222-11	1.528-11
HO2	1.2030-8	9.760-10
H2	2.5750-9	1.594-11
H2O	9.6170-2	9.6177-2
H2O2	4.812-10	5.480-11
H2SO4	2.6999-9	8.1435-8
NO	9.5129-5	1.4919-5
NO2	1.0155-6	5.2640-7
N2	7.3731-1	7.3739-1
N2O	5.6401-9	1.0163-9
NAOH	7.6960-9	1.147-12
NA2SO4	3.1970-8	6.951-11
O	3.5190-9	1.979-11
OH	1.5463-6	5.5734-8
O2	6.7198-2	6.7183-2
O3	1.922-12	1.016-13
SO2	3.6393-4	2.4336-4
SO3	3.0799-5	1.5126-4
M, MOL WT	28.880	28.882
PHASE FRACTION	1.0000 0	1.0000 0
SOLUTION 2		
NAOH(L)	6.3758-6	5.0295-8
NA2SO3(S)	0.000 0	5.620-12
NA2SO3(L)	1.7299-9	0.000000
NA2SO4(I)	0.000000	6.2005-1
NA2SO4(L)	4.8135-1	0.000000
NA2V2O6(L)	5.1653-1	2.2165-1
NA4V2O7(S)	1.8436-4	6.4143-8
NA6V2O8(S)	3.205-10	0.000 0
V2O3(S)	5.9600-9	2.3294-9
V2O5(L)	1.9332-3	1.5830-1
M, MOL WT	194.74	170.91
PHASE FRACTION	2.3725-7	3.2387-7

PURE SPECIES PHASE FRACTIONS (IF ANY)

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-11 FOR ALL ASSIGNED CONDITI

SOLUTION 1

C	CH	CH2	CH2O	CH2O2	CH3	CH2OH	CH3O	CH4	CH
CN	CN2	CNN	COS	CS	CS2	C2	C2H	C2H2	C2
C2H4	C2H4O2	C2H4O4	C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3	C2N	C2
C2O	C3	C3H6O	N-C3H7	I-C3H7	C3H8	1-C3H7OH	C3O2	C4	C4
N-C4H10	I-C4H10	C4N2	C5	C5H5	C5H5O	C6H6	C6H5OH	C7H8	C8
N-C8H18	I-C8H18	O-C12H9	C12H10	HCN	HCO	HNCO	H2N2	H2S	N
NCO	NH	NH2	NH3	NO3	N2H4	N2O4	N2O5	NS	NA
NACN	NAH	NAO	NA2	NA2C2N2	NA2O	NA2O2N2	S	SH	SN
SO	S2	S2O	S8	V	VN	VO	VO2		

SOLUTION 2

NAOH(A)	NA2O(C)	NA2O(A)	NA2O(L)	NA2SO4(IV)	NA2V2O6(S)	NA6V2O8(L)	V2O3(L)	V2O5(S)

PURE SPECIES

C(GR)	C7H8(L)	C8H18(L)	H2O(S)	H2O(L)	H2SO4(L)	VN(S)	N2H6SO4(S)	NA(S)	NA
NACN(S)	NACN(L)	NAO2(S)	NA2CO3(1)	NA2CO3(2)	NA2CO3(L)	NA2O2(A)	NA2O2(B)	NA2S(1)	NA
NA2S(L)	S(S)	S(L)	V(S)	V(L)	NAV3O8(S)	NA2V12O31(S)	NA2V12O31(L)	VO(S)	VO
VO2(S)	VO2(S)	VO2(L)							

STOP

Appendix B. CFBL calculations of Na_2SO_4 deposition rates for selected fuel impurity levels from Table 2. Calculations are repeated for two different wall temperatures, 977 and 1172K.

CFBL THEORY FOR SODIUM SULFATE DEPOSITION RATE

CASE NO. 8701 131 0.1 ppm Na, 1%S, 0.1 ppm V V1ROP1HT

- - INPUT PARAMETERS - - (ALL GAS PROPERTIES PERTAIN TO TJ,PJ)

RUN = 19 TYPE = 0
TO (K) = 1806.000 PO (ATM) = 1.068000
TW (K) = 1172.000 PJ (ATM) = 1.000000
Fuel/Air Mass Ratio (F) = 0.045380
Air Flow Rate (WA, G/SEC) = 2.94000
Dia. Cyl. Target (DIAW, CM) = 0.31800
Length (hgt) Target (LW, CM) = 3.81000
Dia. Jet Nozzle (DJ, CM) = 6.03300
Observed Deposition rate (WOBS, MG/HR) = 0.0045
FSORET? = T

OPTIONAL PARAMETERS
Nozzle Discharge Coef (DC) = 1.000000
SHAPE = 0.0000 DIV = 0.0000
TURBULANCE
TURB = 0.0000
TURIN = 0.0000 PERCENT
TURL (CM) = 0.00000

I=1=NAOH , I=2=NA , I=3=NA2SO4 , I=6=NACL

I	D(I)	NU(I)	SC(I)	X(I),	J X(I),W	TAU(I)	F(SORET),I	M(I)
1	0.27773E+01	0.39893E+01	0.10853E+01	0.50180E-08	0.13280E-08	0.45016E-01	1.02268	0.89010E-03
2	0.35112E+01	0.36321E+01	0.85843E+00	0.41340E-09	0.00000E+00	-0.15846E-01	0.99210	0.10953E-03
3	0.17005E+01	0.48542E+01	0.17725E+01	0.14160E-16	0.95190E-09	0.17019E+00	1.08751	-0.29915E-03
6	0.23382E+01	0.42736E+01	0.12891E+01	0.00000E+00	0.00000E+00	0.92532E-01	1.04698	0.00000E+00

YNAJ	YNAW	YSJ	YSW
0.543140E-08	0.323180E-08	0.394772E-03	0.394881E-03

Average Molec. Wt.= 28.81275
Turbulance factor = 1.00000
Re(EFF) = 57.533
Total Na mass flux to surface (SUM, G/CM**2/SEC) = 1.65482E-11
Total S mass flux to surface (SMS, G/CM**2/SEC) = 3.92336E-07
Na-to-S molar flux ratio at the surface = 0.0001

PREDICTED NA2SO4 DEPOSITION RATE (MG/HR) = 7.00474E-04
ERROR (%) = -8.443E+01

GM = 1.26949
TJ (K) = 1780.95
PR = 0.690190
MOLE FRACTIONS
X(N2) = 0.755099
X(O2) = 0.065770
X(H2O) = 0.089565
X(CO2) = 0.089565

RHOJ(G/CM**3)	UJ(CM/S)	ETAMIX(POISE)	LAMIX(CAL/CM/K/S)	CMIX(CAL/G/S)
0.197159E-03	0.545317E+03	0.594261E-03	0.279215E-03	0.324288E+00

CFBL THEORY FOR SODIUM SULFATE DEPOSITION RATE

NO. 8701 231 1.0 ppm Na, 1%S, 0.1 ppm V V1ROP1HT

- - INPUT PARAMETERS - - (ALL GAS PROPERTIES PERTAIN TO TJ,PJ)

RUN = 19 TYPE = 0

TO (K) = 1806.000 PO (ATM) = 1.068000

TW (K) = 1172.000 PJ (ATM) = 1.000000

Fuel/Air Mass Ratio (F) = 0.045380

Air Flow Rate (WA, G/SEC) = 2.94000

Dia. Cyl. Target (DIAW, CM) = 0.31800

Length (hgt) Target (LW, CM) = 3.81000

Dia. Jet Nozzle (DJ, CM) = 6.03300

Observed Deposition rate (WOBS, MG/HR) = 0.0045

FSORET? = T

OPTIONAL PARAMETERS

Nozzle Discharge Coef (DC) = 1.000000

SHAPE = 0.0000 DIV = 0.0000

TURBULANCE

TURB = 0.0000

TURIN = 0.0000 PERCENT

TURL (CM) = 0.00000

I=1=NAOH , I=2=NA , I=3=NA2SO4 , I=6=NACL

D(I)	NU(I)	SC(I)	X(I),	J X(I),W	TAU(I)	F(SORET),I	M(I)
0.27773E+01	0.39893E+01	0.10853E+01	0.50180E-07	0.64140E-08	0.45016E-01	1.02268	0.10455E-01
0.35112E+01	0.36321E+01	0.85843E+00	0.41340E-08	0.00000E+00	-0.15846E-01	0.99210	0.10953E-02
0.17005E+01	0.48542E+01	0.17725E+01	0.14160E-14	0.22220E-07	0.17019E+00	1.08751	-0.69830E-02
0.23382E+01	0.42736E+01	0.12891E+01	0.00000E+00	0.00000E+00	0.92532E-01	1.04698	0.00000E+00

YNAJ	YNAW	YSJ	YSW
.543140E-07	0.508540E-07	0.394772E-03	0.394880E-03

Average Molec. Wt.= 28.81275

Turbulance factor = 1.00000

Re(EFF) = 57.533

Total Na mass flux to surface (SUM, G/CM**2/SEC) = 1.07891E-10

Total S mass flux to surface (SMS, G/CM**2/SEC) = 3.92381E-07

Na-to-S molar flux ratio at the surface = 0.0004

PREDICTED NA2SO4 DEPOSITION RATE (MG/HR) = 4.56697E-03

ERROR (%) = 1.488E+00

GM = 1.26949

TJ (K) = 1780.95

PR = 0.690190

MOLE FRACTIONS

X(N2) = 0.755099

X(O2) = 0.065770

X(H2O) = 0.089565

X(CO2) = 0.089565

HOJ(G/CM**3)	UJ(CM/S)	ETAMIX(POISE)	LAMIX(CAL/CM/K/S)	CMIX(CAL/G/S)
.197159E-03	0.545317E+03	0.594261E-03	0.279215E-03	0.324288E+00

CFBL THEORY FOR SODIUM SULFATE DEPOSITION RATE

CASE NO. 8701 331 10 ppm Na, 1%S, 0.1 ppm V V1R0P1HT

- - INPUT PARAMETERS - - (ALL GAS PROPERTIES PERTAIN TO TJ,PJ)

RUN = 19 TYPE = 0

TO (K) = 1806.000 PO (ATM) = 1.068000
TW (K) = 1172.000 PJ (ATM) = 1.000000
Fuel/Air Mass Ratio (F) = 0.045380
Air Flow Rate (WA, G/SEC) = 2.94000
Dia. Cyl. Target (DIAW, CM) = 0.31800
Length (hgt) Target (LW, CM) = 3.81000
Dia. Jet Nozzle (DJ, CM) = 6.03300
Observed Deposition rate (WOBS, MG/HR) = 0.0045
FSORET? = T

OPTIONAL PARAMETERS
Nozzle Discharge Coef (DC) = 1.000000
SHAPE = 0.0000 DIV = 0.0000
TURBULANCE
TURB = 0.0000
TURIN = 0.0000 PERCENT
TURL (CM) = 0.00000

I=1=NAOH , I=2=NA , I=3=NA2SO4 , I=6=NACL

I	D(I)	NU(I)	SC(I)	X(I),	J X(I),W	TAU(I)	F(SORET),I	M(I)
1	0.27773E+01	0.39893E+01	0.10853E+01	0.50180E-06	0.11060E-07	0.45016E-01	1.02268	0.11656E+00
2	0.35112E+01	0.36321E+01	0.85843E+00	0.41340E-07	0.14310E-11	-0.15846E-01	0.99210	0.10952E-01
3	0.17005E+01	0.48542E+01	0.17725E+01	0.14160E-12	0.66020E-07	0.17019E+00	1.08751	-0.20748E-01
6	0.23382E+01	0.42736E+01	0.12891E+01	0.00000E+00	0.00000E+00	0.92532E-01	1.04698	0.00000E+00

YNAJ	YNAW	YSJ	YSW
0.543140E-06	0.143101E-06	0.394762E-03	0.394675E-03

Average Molec. Wt.= 28.81275
Turbulance factor = 1.00000
Re(EFF) = 57.533
Total Na mass flux to surface (SUM, G/CM**2/SEC) = 2.52220E-09
Total S mass flux to surface (SMS, G/CM**2/SEC) = 3.93834E-07
Na-to-S molar flux ratio at the surface = 0.0089

PREDICTED NA2SO4 DEPOSITION RATE (MG/HR) = 1.06763E-01
ERROR (%) = 2.273E+03

GM = 1.26949
TJ (K) = 1780.95
PR = 0.690190
MOLE FRACTIONS
X(N2) = 0.755099
X(O2) = 0.065770
X(H2O) = 0.089565
X(CO2) = 0.089565

RHOJ(G/CM**3)	UJ(CM/S)	ETAMIX(POISE)	LAMIX(CAL/CM/K/S)	CMIX(CAL/G/S)
0.197159E-03	0.545317E+03	0.594261E-03	0.279215E-03	0.324288E+00

CFBL THEORY FOR SODIUM SULFATE DEPOSITION RATE

CASE NO. 8701 132 0.1 ppm Na, 1%S, 1.0 ppm V V1ROP1HT

- - INPUT PARAMETERS - - (ALL GAS PROPERTIES PERTAIN TO TJ,PJ)

RUN = 19 TYPE = 0
TO (K) = 1806.000 PO (ATM) = 1.068000
TW (K) = 1172.000 PJ (ATM) = 1.000000
Fuel/Air Mass Ratio (F) = 0.045380
Air Flow Rate (WA, G/SEC) = 2.94000
Dia. Cyl. Target (DIAW, CM) = 0.31800
Length (hgt) Target (LW, CM) = 3.81000
Dia. Jet Nozzle (DJ, CM) = 6.03300
Observed Deposition rate (WOBS, MG/HR) = 0.0045
FSORET? = T

OPTIONAL PARAMETERS
Nozzle Discharge Coef (DC) = 1.000000
SHAPE = 0.0000 DIV = 0.0000
TURBULANCE
TURB = 0.0000
TURIN = 0.0000 PERCENT
TURL (CM) = 0.00000

I=1=NAOH , I=2=NA , I=3=NA2SO4 , I=6=NACL

I	D(I)	NU(I)	SC(I)	X(I),	J X(I),W	TAU(I)	F(SORET),I	M(I)
1	0.27773E+01	0.39893E+01	0.10853E+01	0.50180E-08	0.24180E-09	0.45016E-01	1.02268	0.11359E-02
2	0.35112E+01	0.36321E+01	0.85843E+00	0.41340E-09	0.00000E+00	-0.15846E-01	0.99210	0.10953E-03
3	0.17005E+01	0.48542E+01	0.17725E+01	0.14160E-16	0.31580E-10	0.17019E+00	1.08751	-0.99245E-05
6	0.23382E+01	0.42736E+01	0.12891E+01	0.00000E+00	0.00000E+00	0.92532E-01	1.04698	0.00000E+00

YNAJ	YNAW	YSJ	YSW
0.543140E-08	0.304960E-09	0.394772E-03	0.394880E-03

Average Molec. Wt.= 28.81275
Turbulance factor = 1.00000
Re(EFF) = 57.533
Total Na mass flux to surface (SUM, G/CM**2/SEC) = 2.91878E-11
Total S mass flux to surface (SMS, G/CM**2/SEC) = 3.92340E-07
Na-to-S molar flux ratio at the surface = 0.0001

PREDICTED NA2SO4 DEPOSITION RATE (MG/HR) = 1.23550E-03
ERROR (%) = -7.254E+01

GM = 1.26949
TJ (K) = 1780.95
PR = 0.690190
MOLE FRACTIONS
X(N2) = 0.755099
X(O2) = 0.065770
X(H2O) = 0.089565
X(CO2) = 0.089565

RHOJ(G/CM**3)	UJ(CM/S)	ETAMIX(POISE)	LAMIX(CAL/CM/K/S)	CMIX(CAL/G/S)
0.197159E-03	0.545317E+03	0.594261E-03	0.279215E-03	0.324288E+00

CFBL THEORY FOR SODIUM SULFATE DEPOSITION RATE

CASE NO. 8701 232 1.0 ppm Na, 1%S, 1.0 ppm V V1ROP1HT

- - INPUT PARAMETERS - - (ALL GAS PROPERTIES PERTAIN TO TJ,PJ)

RUN = 19 TYPE = 0
TO (K) = 1806.000 PO (ATM) = 1.068000
TW (K) = 1172.000 PJ (ATM) = 1.000000
Fuel/Air Mass Ratio (F) = 0.045380
Air Flow Rate (WA, G/SEC) = 2.94000
Dia. Cyl. Target (DIAW, CM) = 0.31800
Length (hgt) Target (LW, CM) = 3.81000
Dia. Jet Nozzle (DJ, CM) = 6.03300
Observed Deposition rate (WOBS, MG/HR) = 0.0045
FSORET? = T

OPTIONAL PARAMETERS
Nozzle Discharge Coef (DC) = 1.000000
SHAPE = 0.0000 DIV = 0.0000
TURBULANCE
TURB = 0.0000
TURIN = 0.0000 PERCENT
TURL (CM) = 0.00000

I=1=NAOH , I=2=NA , I=3=NA2SO4 , I=6=NACL

I	D(I)	NU(I)	SC(I)	X(I),	J X(I),W	TAU(I)	F(SORET),I	M(I)
1	0.27773E+01	0.39893E+01	0.10853E+01	0.50180E-07	0.44220E-08	0.45016E-01	1.02268	0.10905E-01
2	0.35112E+01	0.36321E+01	0.85843E+00	0.41340E-08	0.00000E+00	-0.15846E-01	0.99210	0.10953E-02
3	0.17005E+01	0.48542E+01	0.17725E+01	0.14160E-14	0.10560E-07	0.17019E+00	1.08751	-0.33186E-02
6	0.23382E+01	0.42736E+01	0.12891E+01	0.00000E+00	0.00000E+00	0.92532E-01	1.04698	0.00000E+00

YNAJ	YNAW	YSJ	YSW
0.543140E-07	0.255420E-07	0.394772E-03	0.394880E-03

Average Molec. Wt.= 28.81275
Turbulance factor = 1.00000
Re(EFF) = 57.533
Total Na mass flux to surface (SUM, G/CM**2/SEC) = 2.05108E-10
Total S mass flux to surface (SMS, G/CM**2/SEC) = 3.92364E-07
Na-to-S molar flux ratio at the surface = 0.0007

PREDICTED NA2SO4 DEPOSITION RATE (MG/HR) = 8.68209E-03
ERROR (%) = 9.294E+01

GM = 1.26949
TJ (K) = 1780.95
PR = 0.690190
MOLE FRACTIONS
X(N2) = 0.755099
X(O2) = 0.065770
X(H2O) = 0.089565
X(CO2) = 0.089565

RHOJ(G/CM**3)	UJ(CM/S)	ETAMIX(POISE)	LAMIX(CAL/CM/K/S)	CMIX(CAL/G/S)
0.197159E-03	0.545317E+03	0.594261E-03	0.279215E-03	0.324288E+00

CFBL THEORY FOR SODIUM SULFATE DEPOSITION RATE

CASE NO. 8701 332 10. ppm Na, 1%S, 1.0 ppm V V1ROP1HT

- - INPUT PARAMETERS - - (ALL GAS PROPERTIES PERTAIN TO TJ,PJ)

RUN = 19 TYPE = 0
TO (K) = 1806.000 PO (ATM) = 1.068000
TW (K) = 1172.000 PJ (ATM) = 1.000000
Fuel/Air Mass Ratio (F) = 0.045380
Air Flow Rate (WA, G/SEC) = 2.94000
Dia. Cyl. Target (DIAW, CM) = 0.31800
Length (hgt) Target (LW, CM) = 3.81000
Dia. Jet Nozzle (DJ, CM) = 6.03300
Observed Deposition rate (WOBS, MG/HR) = 0.0045
FSORET? = T

OPTIONAL PARAMETERS
Nozzle Discharge Coef (DC) = 1.000000
SHAPE = 0.0000 DIV = 0.0000
TURBULANCE
TURB = 0.0000
TURIN = 0.0000 PERCENT
TURL (CM) = 0.00000

I=1=NAOH , I=2=NA , I=3=NA2SO4 , I=6=NACL

I	D(I)	NU(I)	SC(I)	X(I),	J X(I),W	TAU(I)	F(SORET),I	M(I)
1	0.27773E+01	0.39893E+01	0.10853E+01	0.50180E-06	0.10760E-07	0.45016E-01	1.02268	0.11663E+00
2	0.35112E+01	0.36321E+01	0.85843E+00	0.41340E-07	0.13920E-11	-0.15846E-01	0.99210	0.10952E-01
3	0.17005E+01	0.48542E+01	0.17725E+01	0.14160E-12	0.62430E-07	0.17019E+00	1.08751	-0.19620E-01
6	0.23382E+01	0.42736E+01	0.12891E+01	0.00000E+00	0.00000E+00	0.92532E-01	1.04698	0.00000E+00

YNAJ	YNAW	YSJ	YSW
0.543140E-06	0.135621E-06	0.394762E-03	0.394682E-03

Average Molec. Wt.= 28.81275
Turbulance factor = 1.00000
Re(EFF) = 57.533
Total Na mass flux to surface (SUM, G/CM**2/SEC) = 2.55046E-09
Total S mass flux to surface (SMS, G/CM**2/SEC) = 3.93775E-07
Na-to-S molar flux ratio at the surface = 0.0090

PREDICTED NA2SO4 DEPOSITION RATE (MG/HR) = 1.07959E-01
ERROR (%) = 2.299E+03

GM = 1.26949
TJ (K) = 1780.95
PR = 0.690190
MOLE FRACTIONS
X(N2) = 0.755099
X(O2) = 0.065770
X(H2O) = 0.089565
X(CO2) = 0.089565

RHOJ(G/CM**3)	UJ(CM/S)	ETAMIX(POISE)	LAMIX(CAL/CM/K/S)	CMIX(CAL/G/S)
0.197159E-03	0.545317E+03	0.594261E-03	0.279215E-03	0.324288E+00

CFBL THEORY FOR SODIUM SULFATE DEPOSITION RATE

CASE NO. 8701 133 0.1 ppm Na, 1%S, 10. ppm V V1R0P1HT

- - INPUT PARAMETERS - - (ALL GAS PROPERTIES PERTAIN TO TJ,PJ)

RUN = 19 TYPE = 0
TO (K) = 1806.000 PO (ATM) = 1.068000
TW (K) = 1172.000 PJ (ATM) = 1.000000
Fuel/Air Mass Ratio (F) = 0.045380
Air Flow Rate (WA, G/SEC) = 2.94000
Dia. Cyl. Target (DIAW, CM) = 0.31800
Length (hgt) Target (LW, CM) = 3.81000
Dia. Jet Nozzle (DJ, CM) = 6.03300
Observed Deposition rate (WOBS, MG/HR) = 0.0045
FSORET? = T

OPTIONAL PARAMETERS
Nozzle Discharge Coef (DC) = 1.000000
SHAPE = 0.0000 DIV = 0.0000
TURBULANCE
TURB = 0.0000
TURIN = 0.0000 PERCENT
TURL (CM) = 0.00000

I=1=NAOH , I=2=NA , I=3=NA2SO4 , I=6=NACL

I	D(I)	NU(I)	SC(I)	X(I),	J X(I),W	TAU(I)	F(SORET),I	M(I)
1	0.27773E+01	0.39893E+01	0.10853E+01	0.50180E-08	0.70300E-10	0.45016E-01	1.02268	0.11747E-02
2	0.35112E+01	0.36321E+01	0.85843E+00	0.41340E-09	0.00000E+00	-0.15846E-01	0.99210	0.10953E-03
3	0.17005E+01	0.48542E+01	0.17725E+01	0.14160E-16	0.26690E-11	0.17019E+00	1.08751	-0.83877E-06
6	0.23382E+01	0.42736E+01	0.12891E+01	0.00000E+00	0.00000E+00	0.92532E-01	1.04698	0.00000E+00

YNAJ	YNAW	YSJ	YSW
0.543140E-08	0.756380E-10	0.394762E-03	0.394880E-03

Average Molec. Wt.= 28.81275
Turbulance factor = 1.00000
Re(EFF) = 57.533
Total Na mass flux to surface (SUM, G/CM**2/SEC) = 3.03192E-11
Total S mass flux to surface (SMS, G/CM**2/SEC) = 3.92260E-07
Na-to-S molar flux ratio at the surface = 0.0001

PREDICTED NA2SO4 DEPOSITION RATE (MG/HR) = 1.28339E-03
ERROR (%) = -7.148E+01

GM = 1.26949
TJ (K) = 1780.95
PR = 0.690190
MOLE FRACTIONS
X(N2) = 0.755099
X(O2) = 0.065770
X(H2O) = 0.089565
X(CO2) = 0.089565

RHOJ(G/CM**3)	UJ(CM/S)	ETAMIX(POISE)	LAMIX(CAL/CM/K/S)	CMIX(CAL/G/S)
0.197159E-03	0.545317E+03	0.594261E-03	0.279215E-03	0.324288E+00

CFBL THEORY FOR SODIUM SULFATE DEPOSITION RATE

CASE NO: 8701 233 1.0 ppm Na, 1%S, 10. ppm V V1ROP1HT

- - INPUT PARAMETERS - - (ALL GAS PROPERTIES PERTAIN TO TJ,PJ)

RUN = 19 TYPE = 0

TO (K) = 1806.000 PO (ATM) = 1.068000

TW (K) = 1172.000 PJ (ATM) = 1.000000

Fuel/Air Mass Ratio (F) = 0.045380

Air Flow Rate (WA, G/SEC) = 2.94000

Dia. Cyl. Target (DIAW, CM) = 0.31800

Length (hgt) Target (LW, CM) = 3.81000

Dia. Jet Nozzle (DJ, CM) = 6.03300

Observed Deposition rate (WOBS, MG/HR) = 0.0045

FSORET? = T

OPTIONAL PARAMETERS

Nozzle Discharge Coef (DC) = 1.000000

SHAPE = 0.0000 DIV = 0.0000

TURBULANCE

TURB = 0.0000

TURIN = 0.0000 PERCENT

TURL (CM) = 0.00000

I=1=NAOH , I=2=NA , I=3=NA2SO4 , I=6=NACL

I	D(I)	NU(I)	SC(I)	X(I),	J X(I),W	TAU(I)	F(SORET),I	M(I)
1	0.27773E+01	0.39893E+01	0.10853E+01	0.50180E-07	0.24990E-09	0.45016E-01	1.02268	0.11850E-01
2	0.35112E+01	0.36321E+01	0.85843E+00	0.41340E-08	0.00000E+00	-0.15846E-01	0.99210	0.10953E-02
3	0.17005E+01	0.48542E+01	0.17725E+01	0.14160E-14	0.33720E-10	0.17019E+00	1.08751	-0.10597E-04
6	0.23382E+01	0.42736E+01	0.12891E+01	0.00000E+00	0.00000E+00	0.92532E-01	1.04698	0.00000E+00

YNAJ	YNAW	YSJ	YSW
-0.543140E-07	0.317340E-09	0.394762E-03	0.394880E-03

Average Molec. Wt.= 28.81275

Turbulance factor = 1.00000

Re(EFF) = 57.533

Total Na mass flux to surface (SUM, G/CM**2/SEC) = 3.05563E-10

Total S mass flux to surface (SMS, G/CM**2/SEC) = 3.92260E-07

Na-to-S molar flux ratio at the surface = 0.0011

PREDICTED NA2SO4 DEPOSITION RATE (MG/HR) = 1.29343E-02

ERROR (%) = 1.874E+02

GM = 1.26949

TJ (K) = 1780.95

PR = 0.690190

MOLE FRACTIONS

X(N2) = 0.755099

X(O2) = 0.065770

X(H2O) = 0.089565

X(CO2) = 0.089565

RHOJ(G/CM**3)	UJ(CM/S)	ETAMIX(POISE)	LAMIX(CAL/CM/K/S)	CMIX(CAL/G/S)
0.197159E-03	0.545317E+03	0.594261E-03	0.279215E-03	0.324288E+00

CFBL THEORY FOR SODIUM SULFATE DEPOSITION RATE

CASE NO: 8701 333 10. ppm Na, 1%S, 10. ppm V V1R0P1HT

- - INPUT PARAMETERS - - (ALL GAS PROPERTIES PERTAIN TO TJ,PJ)

RUN = 19 TYPE = 0
TO (K) = 1806.000 PO (ATM) = 1.068000
TW (K) = 1172.000 PJ (ATM) = 1.000000
Fuel/Air Mass Ratio (F) = 0.045380
Air Flow Rate (WA, G/SEC) = 2.94000
Dia. Cyl. Target (DIAW, CM) = 0.31800
Length (hgt) Target (LW, CM) = 3.81000
Dia. Jet Nozzle (DJ, CM) = 6.03300
Observed Deposition rate (WOBS, MG/HR) = 0.0045
FSORET? = T

OPTIONAL PARAMETERS
Nozzle Discharge Coef (DC) = 1.000000
SHAPE = 0.0000 DIV = 0.0000
TURBULANCE
TURB = 0.0000
TURIN = 0.0000 PERCENT
TURL (CM) = 0.00000

I=1=NAOH , I=2=NA , I=3=NA2SO4 , I=6=NACL

I	D(I)	NU(I)	SC(I)	X(I),W	J X(I),W	TAU(I)	F(SORET),I	M(I)
1	0.27773E+01	0.39893E+01	0.10853E+01	0.50180E-06	0.76960E-08	0.45016E-01	1.02268	0.11732E+00
2	0.35112E+01	0.36321E+01	0.85843E+00	0.41340E-07	0.00000E+00	-0.15846E-01	0.99210	0.10953E-01
3	0.17005E+01	0.48542E+01	0.17725E+01	0.14160E-12	0.31970E-07	0.17019E+00	1.08751	-0.10047E-01
6	0.23382E+01	0.42736E+01	0.12891E+01	0.00000E+00	0.00000E+00	0.92532E-01	1.04698	0.00000E+00

YNAJ	YNAW	YSJ	YSW
0.543140E-06	0.716360E-07	0.394762E-03	0.394761E-03

Average Molec. Wt.= 28.81275
Turbulance factor = 1.00000
Re(EFF) = 57.533
Total Na mass flux to surface (SUM, G/CM**2/SEC) = 2.79299E-09
Total S mass flux to surface (SMS, G/CM**2/SEC) = 3.93162E-07
Na-to-S molar flux ratio at the surface = 0.0099

PREDICTED NA2SO4 DEPOSITION RATE (MG/HR) = 1.18225E-01
ERROR (%) = 2.527E+03

GM = 1.26949
TJ (K) = 1780.95
PR = 0.690190
MOLE FRACTIONS
X(N2) = 0.755099
X(O2) = 0.065770
X(H2O) = 0.089565
X(CO2) = 0.089565

RHOJ(G/CM**3)	UJ(CM/S)	ETAMIX(POISE)	LAMIX(CAL/CM/K/S)	CMIX(CAL/G/S)
0.197159E-03	0.545317E+03	0.594261E-03	0.279215E-03	0.324288E+00

CFBL THEORY FOR SODIUM SULFATE DEPOSITION RATE

CASE NO. 8701 131 0.1 ppm Na, 1%S, 0.1 ppm V V1ROP1B.CFB

- - INPUT PARAMETERS - - (ALL GAS PROPERTIES PERTAIN TO TJ,PJ)

RUN = 19 TYPE = 0
TO (K) = 1806.000 PO (ATM) = 1.068000
TW (K) = 977.000 PJ (ATM) = 1.000000
Fuel/Air Mass Ratio (F) = 0.045380
Air Flow Rate (WA, G/SEC) = 2.94000
Dia. Cyl. Target (DIAW, CM) = 0.31800
Length (hgt) Target (LW, CM) = 3.81000
Dia. Jet Nozzle (DJ, CM) = 6.03300
Observed Deposition rate (WOBS, MG/HR) = 0.0045
FSORET? = T

OPTIONAL PARAMETERS
Nozzle Discharge Coef (DC) = 1.000000
SHAPE = 0.0000 DIV = 0.0000
TURBULANCE
TURB = 0.0000
TURIN = 0.0000 PERCENT
TURL (CM) = 0.00000

I=1=NAOH , I=2=NA , I=3=NA2SO4 , I=6=NACL

I	D(I)	NU(I)	SC(I)	X(I),	J X(I),W	TAU(I)	F(SORET),I	M(I)
1	0.27773E+01	0.39604E+01	0.10853E+01	0.50180E-08	0.11390E-11	0.61792E-01	1.03121	0.11916E-02
2	0.35112E+01	0.36058E+01	0.85843E+00	0.41340E-09	0.00000E+00	-0.20278E-01	0.98990	0.10849E-03
3	0.17005E+01	0.48190E+01	0.17725E+01	0.14160E-16	0.68640E-10	0.22782E+00	1.11823	-0.20627E-04
6	0.23382E+01	0.42426E+01	0.12891E+01	0.00000E+00	0.00000E+00	0.12757E+00	1.06514	0.00000E+00

YNAJ	YNAW	YSJ	YSW
0.543140E-08	0.138419E-09	0.394772E-03	0.394830E-03

Average Molec. Wt.= 28.81275
Turbulance factor = 1.00000
Re(EFF) = 57.533
Total Na mass flux to surface (SUM, G/CM**2/SEC) = 3.02262E-11
Total S mass flux to surface (SMS, G/CM**2/SEC) = 6.47981E-07
Na-to-S molar flux ratio at the surface = 0.0001

PREDICTED NA2SO4 DEPOSITION RATE (MG/HR) = 1.27946E-03
ERROR (%) = -7.157E+01

GM = 1.26949
TJ (K) = 1780.95
PR = 0.690190
MOLE FRACTIONS
X(N2) = 0.755099
X(O2) = 0.065770
X(H2O) = 0.089565
X(CO2) = 0.089565

RHOJ(G/CM**3)	UJ(CM/S)	ETAMIX(POISE)	LAMIX(CAL/CM/K/S)	CMIX(CAL/G/S)
0.197159E-03	0.545317E+03	0.594261E-03	0.279215E-03	0.324288E+00

CFBL THEORY FOR SODIUM SULFATE DEPOSITION RATE

CASE NO. 8701 231 1.0 ppm Na, 1%S, 0.1 ppm V V1R0P1B.CFB

- - INPUT PARAMETERS - - (ALL GAS PROPERTIES PERTAIN TO TJ,PJ)

RUN = 19 TYPE = 0
TO (K) = 1806.000 PO (ATM) = 1.068000
TW (K) = 977.000 PJ (ATM) = 1.000000
Fuel/Air Mass Ratio (F) = 0.045380
Air Flow Rate (WA, G/SEC) = 2.94000
Dia. Cyl. Target (DIAW, CM) = 0.31800
Length (hgt) Target (LW, CM) = 3.81000
Dia. Jet Nozzle (DJ, CM) = 6.03300
Observed Deposition rate (WOBS, MG/HR) = 0.0045
FSORET? = T

OPTIONAL PARAMETERS
Nozzle Discharge Coef (DC) = 1.000000
SHAPE = 0.0000 DIV = 0.0000
TURBULANCE
TURB = 0.0000
TURIN = 0.0000 PERCENT
TURL (CM) = 0.00000

I=1=NAOH , I=2=NA , I=3=NA2SO4 , I=6=NACL

I	D(I)	NU(I)	SC(I)	X(I),	J X(I),W	TAU(I)	F(SORET),I	M(I)
1	0.27773E+01	0.39604E+01	0.10853E+01	0.50180E-07	0.14230E-11	0.61792E-01	1.03121	0.11918E-01
2	0.35112E+01	0.36058E+01	0.85843E+00	0.41340E-08	0.00000E+00	-0.20278E-01	0.98990	0.10849E-02
3	0.17005E+01	0.48190E+01	0.17725E+01	0.14160E-14	0.10710E-09	0.22782E+00	1.11823	-0.32183E-04
6	0.23382E+01	0.42426E+01	0.12891E+01	0.00000E+00	0.00000E+00	0.12757E+00	1.06514	0.00000E+00

YNAJ	YNAW	YSJ	YSW
0.543140E-07	0.215623E-09	0.394772E-03	0.394800E-03

Average Molec. Wt.= 28.81275
Turbulance factor = 1.00000
Re(EFF) = 57.533
Total Na mass flux to surface (SUM, G/CM**2/SEC) = 3.06427E-10
Total S mass flux to surface (SMS, G/CM**2/SEC) = 6.48180E-07
Na-to-S molar flux ratio at the surface = 0.0007

PREDICTED NA2SO4 DEPOSITION RATE (MG/HR) = 1.29709E-02
ERROR (%) = 1.882E+02

GM = 1.26949
TJ (K) = 1780.95
PR = 0.690190
MOLE FRACTIONS
X(N2) = 0.755099
X(O2) = 0.065770
X(H2O) = 0.089565
X(CO2) = 0.089565

RHOJ(G/CM**3)	UJ(CM/S)	ETAMIX(POISE)	LAMIX(CAL/CM/K/S)	CMIX(CAL/G/S)
0.197159E-03	0.545317E+03	0.594261E-03	0.279215E-03	0.324288E+00

CFBL THEORY FOR SODIUM SULFATE DEPOSITION RATE

CASE NO. 8701 331 10 ppm Na, 1%S, 0.1 ppm V V1ROP1B.CFB

- - INPUT PARAMETERS - - (ALL GAS PROPERTIES PERTAIN TO TJ,PJ)

RUN = 19 TYPE = 0

TO (K) = 1806.000 PO (ATM) = 1.068000

TW (K) = 977.000 PJ (ATM) = 1.000000

Fuel/Air Mass Ratio (F) = 0.045380

Air Flow Rate (WA, G/SEC) = 2.94000

Dia. Cyl. Target (DIAW, CM) = 0.31800

Length (hgt) Target (LW, CM) = 3.81000

Dia. Jet Nozzle (DJ, CM) = 6.03300

Observed Deposition rate (WOBS, MG/HR) = 0.0045

FSORET? = T

OPTIONAL PARAMETERS

Nozzle Discharge Coef (DC) = 1.000000

SHAPE = 0.0000 DIV = 0.0000

TURBULANCE

TURB = 0.0000

TURIN = 0.0000 PERCENT

TURL (CM) = 0.00000

I=1=NAOH , I=2=NA , I=3=NA2SO4 , I=6=NACL

I	D(I)	NU(I)	SC(I)	X(I),	J X(I),W	TAU(I)	F(SORET),I	M(I)
1	0.27773E+01	0.39604E+01	0.10853E+01	0.50180E-06	0.14530E-11	0.61792E-01	1.03121	0.11918E+00
2	0.35112E+01	0.36058E+01	0.85843E+00	0.41340E-07	0.46440E-17	-0.20278E-01	0.98990	0.10849E-01
3	0.17005E+01	0.48190E+01	0.17725E+01	0.14160E-12	0.11160E-09	0.22782E+00	1.11823	-0.33482E-04
6	0.23382E+01	0.42426E+01	0.12891E+01	0.00000E+00	0.00000E+00	0.12757E+00	1.06514	0.00000E+00

YNAJ	YNAW	YSJ	YSW
0.543140E-06	0.224653E-09	0.394762E-03	0.394560E-03

Average Molec. Wt.= 28.81275

Turbulance factor = 1.00000

Re(EFF) = 57.533

Total Na mass flux to surface (SUM, G/CM**2/SEC) = 3.07115E-09

Total S mass flux to surface (SMS, G/CM**2/SEC) = 6.49682E-07

Na-to-S molar flux-ratio at the surface = 0.0066

PREDICTED NA2SO4 DEPOSITION RATE (MG/HR) = 1.30000E-01

ERROR (%) = 2.789E+03

GM = 1.26949

TJ (K) = 1780.95

PR = 0.690190

MOLE FRACTIONS

X(N2) = 0.755099

X(O2) = 0.065770

X(H2O) = 0.089565

X(CO2) = 0.089565

RHOJ(G/CM**3)	UJ(CM/S)	ETAMIX(POISE)	LAMIX(CAL/CM/K/S)	CMIX(CAL/G/S)
0.197159E-03	0.545317E+03	0.594261E-03	0.279215E-03	0.324288E+00

CFBL THEORY FOR SODIUM SULFATE DEPOSITION RATE

CASE NO. 8701 132 0.1 ppm Na, 1%S, 1.0 ppm V V1R0P1B.CFB

- - INPUT PARAMETERS - - (ALL GAS PROPERTIES PERTAIN TO TJ,PJ)

RUN = 19 TYPE = 0
TO (K) = 1806.000 PO (ATM) = 1.068000
TW (K) = 977.000 PJ (ATM) = 1.000000
Fuel/Air Mass Ratio (F) = 0.045380
Air Flow Rate (WA, G/SEC) = 2.94000
Dia. Cyl. Target (DIAW, CM) = 0.31800
Length (hgt) Target (LW, CM) = 3.81000
Dia. Jet Nozzle (DJ, CM) = 6.03300
Observed Deposition rate (WOBS, MG/HR) = 0.0045
FSORET? = T

OPTIONAL PARAMETERS
Nozzle Discharge Coef (DC) = 1.000000
SHAPE = 0.0000 DIV = 0.0000
TURBULANCE
TURB = 0.0000
TURIN = 0.0000 PERCENT
TURL (CM) = 0.00000

I=1=NAOH , I=2=NA , I=3=NA2SO4 , I=6=NACL

I	D(I)	NU(I)	SC(I)	X(I),	J X(I),W	TAU(I)	F(SORET),I	M(I)
1	0.27773E+01	0.39604E+01	0.10853E+01	0.50180E-08	0.39400E-12	0.61792E-01	1.03121	0.11918E-02
2	0.35112E+01	0.36058E+01	0.85843E+00	0.41340E-09	0.00000E+00	-0.20278E-01	0.98990	0.10849E-03
3	0.17005E+01	0.48190E+01	0.17725E+01	0.14160E-16	0.82120E-11	0.22782E+00	1.11823	-0.24677E-05
6	0.23382E+01	0.42426E+01	0.12891E+01	0.00000E+00	0.00000E+00	0.12757E+00	1.06514	0.00000E+00

YNAJ	YNAW	YSJ	YSW
0.543140E-08	0.168180E-10	0.394772E-03	0.394830E-03

Average Molec. Wt.= 28.81275
Turbulance factor = 1.00000
Re(EFF) = 57.533
Total Na mass flux to surface (SUM, G/CM**2/SEC) = 3.06591E-11
Total S mass flux to surface (SMS, G/CM**2/SEC) = 6.47981E-07
Na-to-S molar flux ratio at the surface = 0.0001

PREDICTED NA2SO4 DEPOSITION RATE (MG/HR) = 1.29778E-03
ERROR (%) = -7.116E+01

GM = 1.26949
TJ (K) = 1780.95
PR = 0.690190
MOLE FRACTIONS
X(N2) = 0.755099
X(O2) = 0.065770
X(H2O) = 0.089565
X(CO2) = 0.089565

RHOJ(G/CM**3)	UJ(CM/S)	ETAMIX(POISE)	LAMIX(CAL/CM/K/S)	CMIX(CAL/G/S)
0.197159E-03	0.545317E+03	0.594261E-03	0.279215E-03	0.324288E+00

CFBL THEORY FOR SODIUM SULFATE DEPOSITION RATE

CASE NO: 8701 232 1.0 ppm Na, 1%S, 1.0 ppm V V1ROP1B.CFB

- - INPUT PARAMETERS - - (ALL GAS PROPERTIES PERTAIN TO TJ,PJ)

RUN = 19 TYPE = 0
TO (K) = 1806.000 PO (ATM) = 1.068000
TW (K) = 977.000 PJ (ATM) = 1.000000
Fuel/Air Mass Ratio (F) = 0.045380
Air Flow Rate (WA, G/SEC) = 2.94000
Dia. Cyl. Target (DIAW, CM) = 0.31800
Length (hgt) Target (LW, CM) = 3.81000
Dia. Jet Nozzle (DJ, CM) = 6.03300
Observed Deposition rate (WOBS, MG/HR) = 0.0045
FSORET? = T

OPTIONAL PARAMETERS
Nozzle Discharge Coef (DC) = 1.000000
SHAPE = 0.0000 DIV = 0.0000
TURBULANCE
TURB = 0.0000
TURIN = 0.0000 PERCENT
TURL (CM) = 0.00000

I=1=NAOH , I=2=NA , I=3=NA2SO4 , I=6=NACL

I	D(I)	NU(I)	SC(I)	X(I),	J X(I),W	TAU(I)	F(SORET),I	M(I)
1	0.27773E+01	0.39604E+01	0.10853E+01	0.50180E-07	0.11460E-11	0.61792E-01	1.03121	0.11918E-01
2	0.35112E+01	0.36058E+01	0.85843E+00	0.41340E-08	0.00000E+00	-0.20278E-01	0.98990	0.10849E-02
3	0.17005E+01	0.48190E+01	0.17725E+01	0.14160E-14	0.69430E-10	0.22782E+00	1.11823	-0.20863E-04
6	0.23382E+01	0.42426E+01	0.12891E+01	0.00000E+00	0.00000E+00	0.12757E+00	1.06514	0.00000E+00

YNAJ	YNAW	YSJ	YSW
0.543140E-07	0.140006E-09	0.394772E-03	0.394800E-03

Average Molec. Wt.= 28.81275
Turbulance factor = 1.00000
Re(EFF) = 57.533
Total Na mass flux to surface (SUM, G/CM**2/SEC) = 3.06696E-10
Total S mass flux to surface (SMS, G/CM**2/SEC) = 6.48180E-07
Na-to-S molar flux ratio at the surface = 0.0007

PREDICTED NA2SO4 DEPOSITION RATE (MG/HR) = 1.29822E-02
ERROR (%) = 1.885E+02

GM = 1.26949
TJ (K) = 1780.95
PR = 0.690190
MOLE FRACTIONS
X(N2) = 0.755099
X(O2) = 0.065770
X(H2O) = 0.089565
X(CO2) = 0.089565

RHOJ(G/CM**3)	UJ(CM/S)	ETAMIX(POISE)	LAMIX(CAL/CM/K/S)	CMIX(CAL/G/S)
0.197159E-03	0.545317E+03	0.594261E-03	0.279215E-03	0.324288E+00

CFBL THEORY FOR SODIUM SULFATE DEPOSITION RATE

ASE NO. 8701 332 10. ppm Na, 1%S, 1.0 ppm V V1R0P1B.CFB

- - INPUT PARAMETERS - - (ALL GAS PROPERTIES PERTAIN TO TJ,PJ)

RUN = 19 TYPE = 0
TO (K) = 1806.000 PO (ATM) = 1.068000
TW (K) = 977.000 PJ (ATM) = 1.000000
Fuel/Air Mass Ratio (F) = 0.045380
Air Flow Rate (WA, G/SEC) = 2.94000
Dia. Cyl. Target (DIAW, CM) = 0.31800
Length (hgt) Target (LW, CM) = 3.81000
Dia. Jet Nozzle (DJ, CM) = 6.03300
Observed Deposition rate (WOBS, MG/HR) = 0.0045
FSORET? = T

OPTIONAL PARAMETERS
Nozzle Discharge Coef (DC) = 1.000000
SHAPE = 0.0000 DIV = 0.0000
TURBULANCE
TURB = 0.0000
TURIN = 0.0000 PERCENT
TURL (CM) = 0.00000

I=1=NAOH , I=2=NA , I=3=NA2SO4 , I=6=NACL

D(I)	NU(I)	SC(I)	X(I),	J X(I),W	TAU(I)	F(SORET),I	M(I)
0.27773E+01	0.39604E+01	0.10853E+01	0.50180E-06	0.14240E-11	0.61792E-01	1.03121	0.11918E+00
0.35112E+01	0.36058E+01	0.85843E+00	0.41340E-07	0.45500E-17	-0.20278E-01	0.98990	0.10849E-01
0.17005E+01	0.48190E+01	0.17725E+01	0.14160E-12	0.10710E-09	0.22782E+00	1.11823	-0.32130E-04
0.23382E+01	0.42426E+01	0.12891E+01	0.00000E+00	0.00000E+00	0.12757E+00	1.06514	0.00000E+00

YNAJ	YNAW	YSJ	YSW
0.543140E-06	0.215624E-09	0.394762E-03	0.394560E-03

Average Molec. Wt.= 28.81275
Turbulance factor = 1.00000
Re(EFF) = 57.533
Total Na mass flux to surface (SUM, G/CM**2/SEC) = 3.07118E-09
Total S mass flux to surface (SMS, G/CM**2/SEC) = 6.49682E-07
Na-to-S molar flux ratio at the surface = 0.0066

PREDICTED NA2SO4 DEPOSITION RATE (MG/HR) = 1.30001E-01
ERROR (%) = 2.789E+03

GM = 1.26949
TJ (K) = 1780.95
PR = 0.690190
MOLE FRACTIONS
X(N2) = 0.755099
X(O2) = 0.065770
X(H2O) = 0.089565
X(CO2) = 0.089565

RHOJ(G/CM**3)	UJ(CM/S)	ETAMIX(POISE)	LAMIX(CAL/CM/K/S)	CMIX(CAL/G/S)
0.197159E-03	0.545317E+03	0.594261E-03	0.279215E-03	0.324288E+00

CFBL THEORY FOR SODIUM SULFATE DEPOSITION RATE

CASE NO. 8701 133 0.1 ppm Na, 1%S, 10. ppm V V1ROP1B.CFB

· · INPUT PARAMETERS · · (ALL GAS PROPERTIES PERTAIN TO TJ,PJ)

RUN = 19 TYPE = 0

TO (K) = 1806.000 PO (ATM) = 1.068000

TW (K) = 977.000 PJ (ATM) = 1.000000

Fuel/Air Mass Ratio (F) = 0.045380

Air Flow Rate (WA, G/SEC) = 2.94000

Dia. Cyl. Target (DIAW, CM) = 0.31800

Length (hgt) Target (LW, CM) = 3.81000

Dia. Jet Nozzle (DJ, CM) = 6.03300

Observed Deposition rate (WOBS, MG/HR) = 0.0045

FSORET? = T

OPTIONAL PARAMETERS

Nozzle Discharge Coef (DC) = 1.000000

SHAPE = 0.0000 DIV = 0.0000

TURBULANCE

TURB = 0.0000

TURIN = 0.0000 PERCENT

TURL (CM) = 0.00000

I=1=NAOH , I=2=NA , I=3=NA2SO4 , I=6=NACL

I	D(I)	NU(I)	SC(I)	X(I),	J X(I),W	TAU(I)	F(SORET),I	M(I)
1	0.27773E+01	0.39604E+01	0.10853E+01	0.50180E-08	0.12060E-12	0.61792E-01	1.03121	0.11918E-02
2	0.35112E+01	0.36058E+01	0.85843E+00	0.41340E-09	0.00000E+00	-0.20278E-01	0.98990	0.10849E-03
3	0.17005E+01	0.48190E+01	0.17725E+01	0.14160E-16	0.76920E-12	0.22782E+00	1.11823	-0.23114E-06
6	0.23382E+01	0.42426E+01	0.12891E+01	0.00000E+00	0.00000E+00	0.12757E+00	1.06514	0.00000E+00

YNAJ	YNAW	YSJ	YSW
0.543140E-08	0.165900E-11	0.394762E-03	0.394820E-03

Average Molec. Wt.= 28.81275

Turbulance factor = 1.00000

Re(EFF) = 57.533

Total Na mass flux to surface (SUM, G/CM**2/SEC) = 3.07134E-11

Total S mass flux to surface (SMS, G/CM**2/SEC) = 6.47967E-07

Na-to-S molar flux ratio at the surface = 0.0001

PREDICTED NA2SO4 DEPOSITION RATE (MG/HR) = 1.30008E-03

ERROR (%) = -7.111E+01

GM = 1.26949

TJ (K) = 1780.95

PR = 0.690190

MOLE FRACTIONS

X(N2) = 0.755099

X(O2) = 0.065770

X(H2O) = 0.089565

X(CO2) = 0.089565

RHOJ(G/CM**3)	UJ(CM/S)	ETAMIX(POISE)	LAMIX(CAL/CM/K/S)	CMIX(CAL/G/S)
0.197159E-03	0.545317E+03	0.594261E-03	0.279215E-03	0.324288E+00

CFBL THEORY FOR SODIUM SULFATE DEPOSITION RATE

CASE NO. 8701 233 1.0 ppm Na, 1%S, 10. ppm V V1R0P1B.CFB

- - INPUT PARAMETERS - - (ALL GAS PROPERTIES PERTAIN TO TJ,PJ)

RUN = 19 TYPE = 0

TO (K) = 1806.000 PO (ATM) = 1.068000

TW (K) = 977.000 PJ (ATM) = 1.000000

Fuel/Air Mass Ratio (F) = 0.045380

Air Flow Rate (WA, G/SEC) = 2.94000

Dia. Cyl. Target (DIAW, CM) = 0.31800

Length (hgt) Target (LW, CM) = 3.81000

Dia. Jet Nozzle (DJ, CM) = 6.03300

Observed Deposition rate (WOBS, MG/HR) = 0.0045

FSORET? = T

OPTIONAL PARAMETERS

Nozzle Discharge Coef (DC) = 1.000000

SHAPE = 0.0000 DIV = 0.0000

TURBULANCE

TURB = 0.0000

TURIN = 0.0000 PERCENT

TURL (CM) = 0.00000

I=1=NAOH , I=2=NA , I=3=NA2SO4 , I=6=NACL

I	D(I)	NU(I)	SC(I)	X(I),	J X(I),W	TAU(I)	F(SORET),I	M(I)
1	0.27773E+01	0.39604E+01	0.10853E+01	0.50180E-07	0.39460E-12	0.61792E-01	1.03121	0.11918E-01
2	0.35112E+01	0.36058E+01	0.85843E+00	0.41340E-08	0.00000E+00	-0.20278E-01	0.98990	0.10849E-02
3	0.17005E+01	0.48190E+01	0.17725E+01	0.14160E-14	0.82360E-11	-0.22782E+00	1.11823	-0.24744E-05
6	0.23382E+01	0.42426E+01	0.12891E+01	0.00000E+00	0.00000E+00	0.12757E+00	1.06514	0.00000E+00

YNAJ	YNAW	YSJ	YSW
0.543140E-07	0.168666E-10	0.394762E-03	0.394820E-03

Average Molec. Wt.= 28.81275

Turbulance factor = 1.00000

Re(EFF) = 57.533

Total Na mass flux to surface (SUM, G/CM**2/SEC) = 3.07135E-10

Total S mass flux to surface (SMS, G/CM**2/SEC) = 6.47967E-07

Na-to-S molar flux ratio at the surface = 0.0007

PREDICTED NA2SO4 DEPOSITION RATE (MG/HR) = 1.30008E-02

ERROR (%) = 1.889E+02

GM = 1.26949

TJ (K) = 1780.95

PR = 0.690190

MOLE FRACTIONS

X(N2) = 0.755099

X(O2) = 0.065770

X(H2O) = 0.089565

X(CO2) = 0.089565

RHOJ(G/CM**3)	UJ(CM/S)	ETAMIX(POISE)	LAMIX(CAL/CM/K/S)	CMIX(CAL/G/S)
0.197159E-03	0.545317E+03	0.594261E-03	0.279215E-03	0.324288E+00

CFBL THEORY FOR SODIUM SULFATE DEPOSITION RATE

CASE NO: 8701 333 10. ppm Na, 1%S, 10. ppm V V1ROP1B.CFB

- - INPUT PARAMETERS - - (ALL GAS PROPERTIES PERTAIN TO TJ,PJ)

RUN = 19 TYPE = 0
TO (K) = 1806.000 PO (ATM) = 1.068000
TW (K) = 977.000 PJ (ATM) = 1.000000
Fuel/Air Mass Ratio (F) = 0.045380
Air Flow Rate (WA, G/SEC) = 2.94000
Dia. Cyl. Target (DIAW, CM) = 0.31800
Length (hgt) Target (LW, CM) = 3.81000
Dia. Jet Nozzle (DJ, CM) = 6.03300
Observed Deposition rate (WOBS, MG/HR) = 0.0045
FSORET? = T

OPTIONAL PARAMETERS
Nozzle Discharge Coef (DC) = 1.000000
SHAPE = 0.0000 DIV = 0.0000
TURBULANCE
TURB = 0.0000
TURIN = 0.0000 PERCENT
TURL (CM) = 0.00000

I=1=NAOH , I=2=NA , I=3=NA2SO4 , I=6=NACL

I	D(I)	NU(I)	SC(I)	X(I),	J X(I),W	TAU(I)	F(SORET),I	M(I)
1	0.27773E+01	0.39604E+01	0.10853E+01	0.50180E-06	0.11470E-11	0.61792E-01	1.03121	0.11918E+00
2	0.35112E+01	0.36058E+01	0.85843E+00	0.41340E-07	0.00000E+00	-0.20278E-01	0.98990	0.10849E-01
3	0.17005E+01	0.48190E+01	0.17725E+01	0.14160E-12	0.69510E-10	0.22782E+00	1.11823	-0.20834E-04
6	0.23382E+01	0.42426E+01	0.12891E+01	0.00000E+00	0.00000E+00	0.12757E+00	1.06514	0.00000E+00

YNAJ	YNAW	YSJ	YSW
0.543140E-06	0.140167E-09	0.394762E-03	0.394620E-03

Average Molec. Wt.= 28.81275
Turbulance factor = 1.00000
Re(EFF) = 57.533
Total Na mass flux to surface (SUM, G/CM**2/SEC) = 3.07145E-09
Total S mass flux to surface (SMS, G/CM**2/SEC) = 6.49285E-07
Na-to-S molar flux ratio at the surface = 0.0066

PREDICTED NA2SO4 DEPOSITION RATE (MG/HR) = 1.30012E-01
ERROR (%) = 2.789E+03

GM = 1.26949
TJ (K) = 1780.95
PR = 0.690190
MOLE FRACTIONS
X(N2) = 0.755099
X(O2) = 0.065770
X(H2O) = 0.089565
X(CO2) = 0.089565

RHOJ(G/CM**3)	UJ(CM/S)	ETAMIX(POISE)	LAMIX(CAL/CM/K/S)	CMIX(CAL/G/S)
0.197159E-03	0.545317E+03	0.594261E-03	0.279215E-03	0.324288E+00

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5. AUTHOR(S)

Lawrence P. Cook and David W. Bonnell

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10. SUPPLEMENTARY NOTES

☐ Document describes a computer program; SF-185, FIPS Software Summary, is attached.

11. ABSTRACT (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here)

An integrated equilibrium kinetic model is described for treating the chemical solution component of corrosion of (Co,Cr)-based superalloys by the (Na, S, V)-molten salts originating from impurities present in hydrocarbon fuels. Gas phase chemistry and gas phase/condensed phase precipitate interactions are modeled using the NASA-Lewis multicomponent free energy minimization program (CEC). Salt deposition rates are calculated with the aid of a chemical frozen boundary layer (CFBL) program. Solubilities of superalloy components (Co and Cr) are modeled from phase equilibrium data, and rate of solution is described by assuming a very thin steady state oxide film, with formation and dissolution occurring according to a parabolic rate law. A range of steady state corrosion rates can be predicted using this approach which are in general agreement with the range of reported test rig results. Further model development would benefit from additional experimental phase equilibrium data on the system Na_2O-CoO-Cr_2O_3-SO_3-V_2O_5.

12. KEY WORDS (Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)

chromium; cobalt; high temperature solubility; hot corrosion; molten salts; sodium; sulfate; sulfur; superalloys, vanadate

13. AVAILABILITY

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